Supporting Information

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Bioactive compounds from the flowers of *Cannabis sativa* L.: Isolation of a new alkaloid and biological evaluation of cannabinoids and sesquiterpenoids

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1. Spectroscopic data for compound 1

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{14}H_{19}NO_3$	250.1438	250.1444	- 2.52 / - 0.63

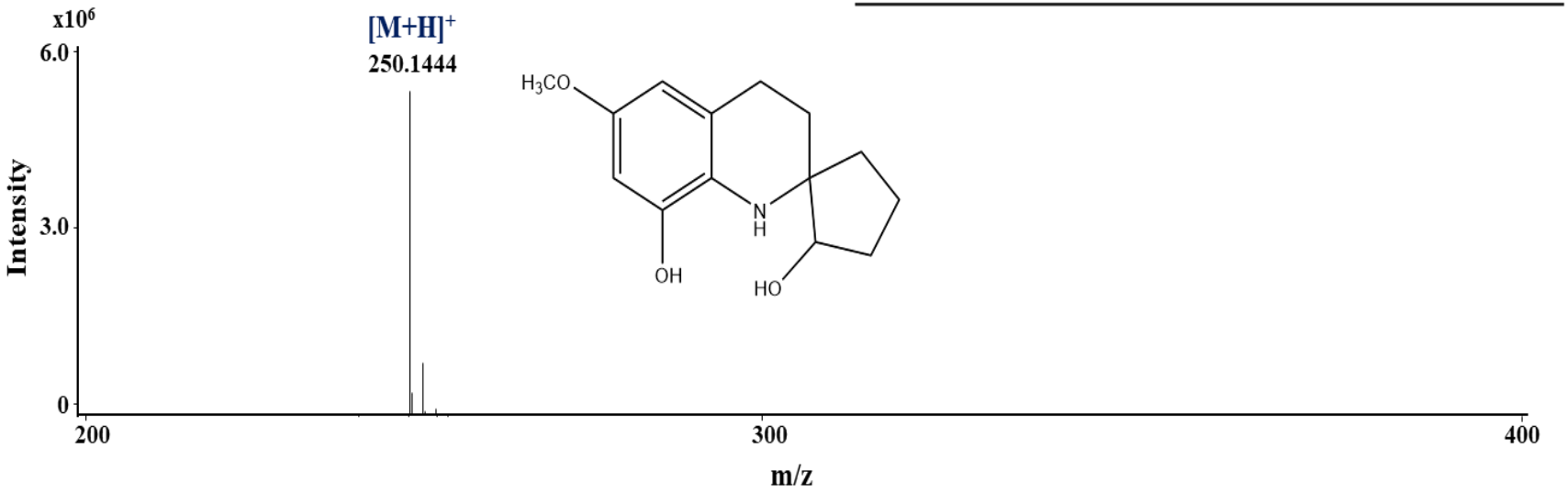


Figure S1. MS spectrum of **1**

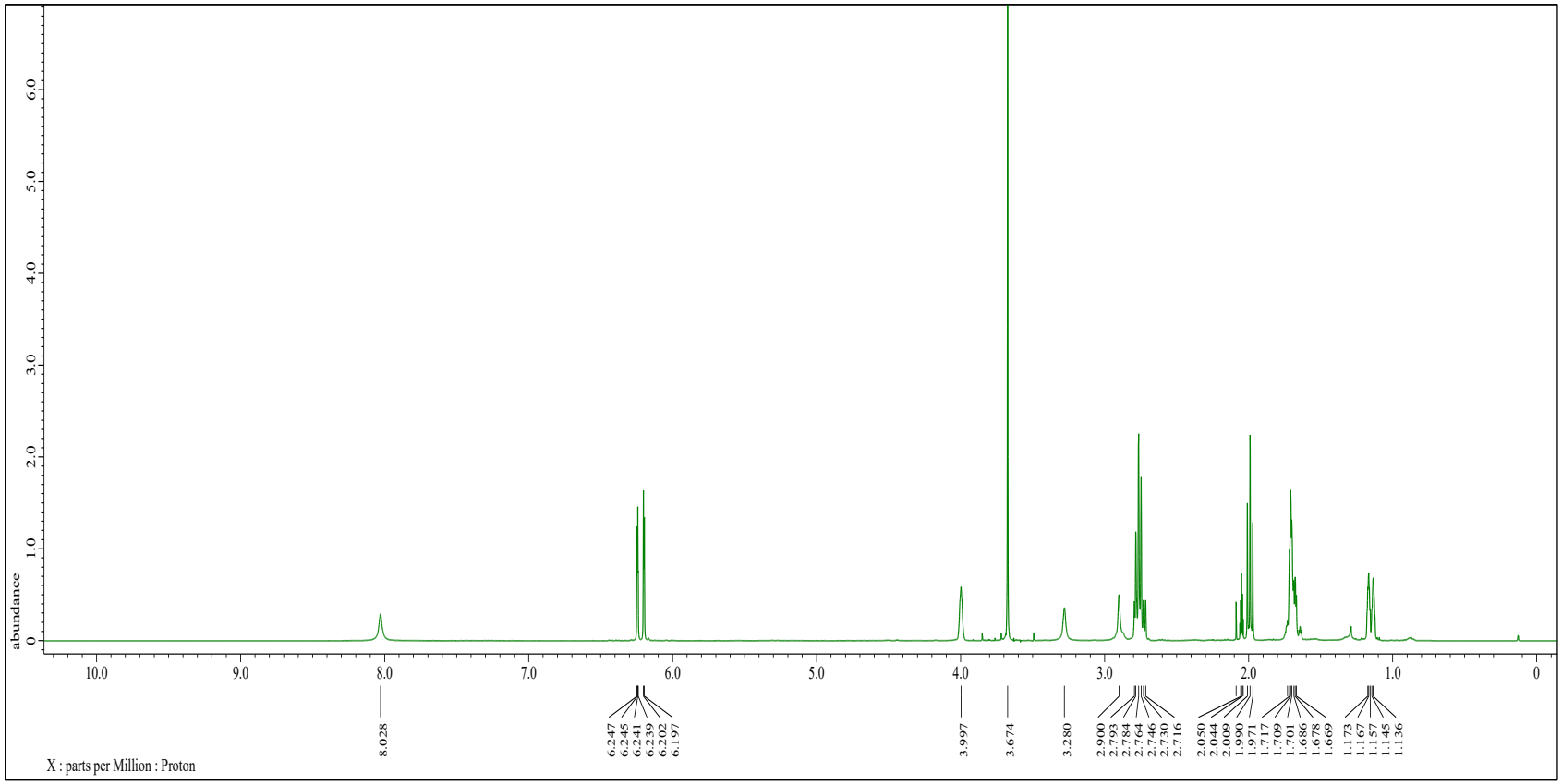


Figure S2. ^{1}H NMR spectrum of **1** (Recorded in Acetone-*d6*)

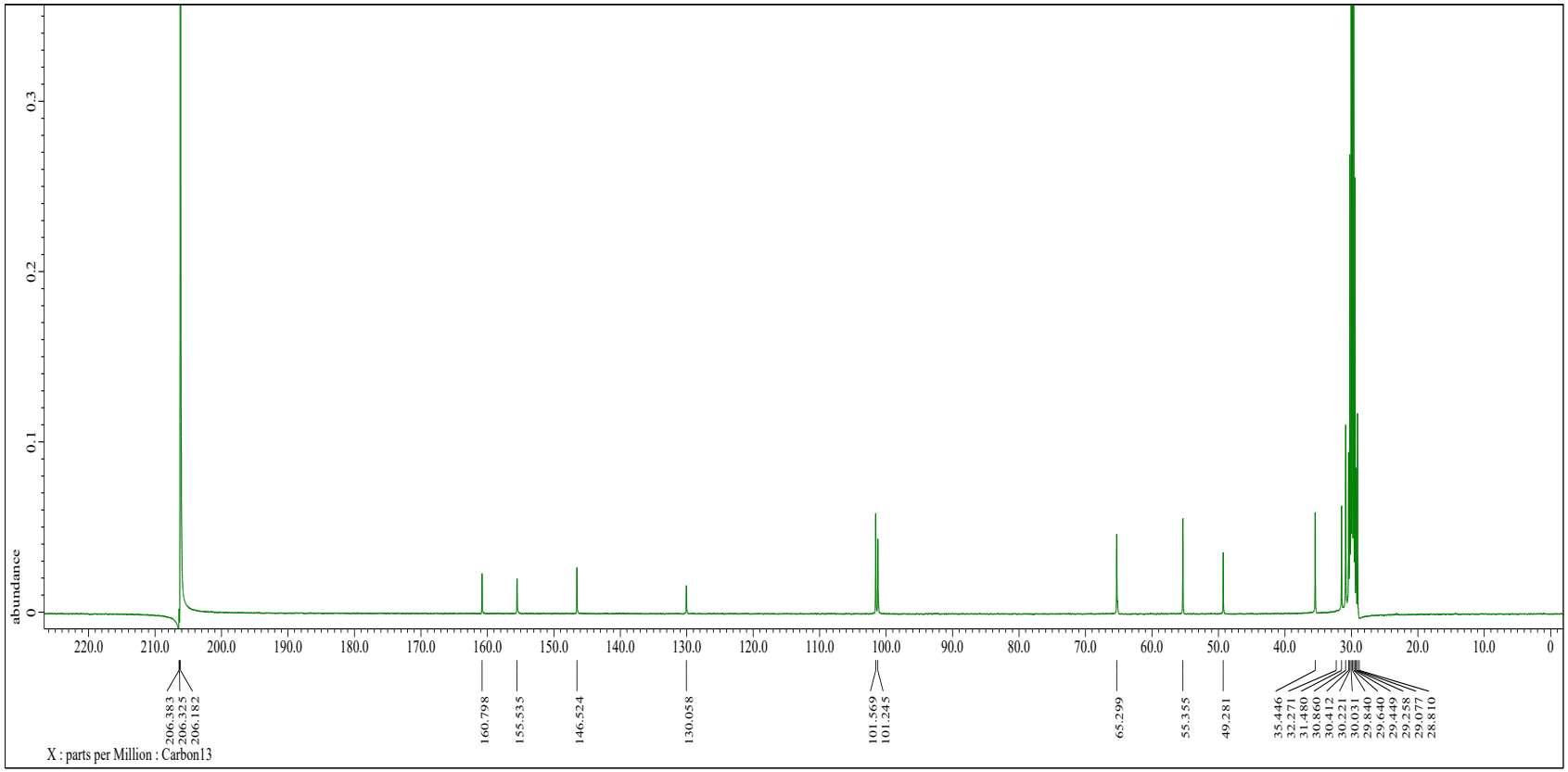


Figure S3. ^{13}C NMR spectrum of **1** (Recorded in Acetone-*d6*)

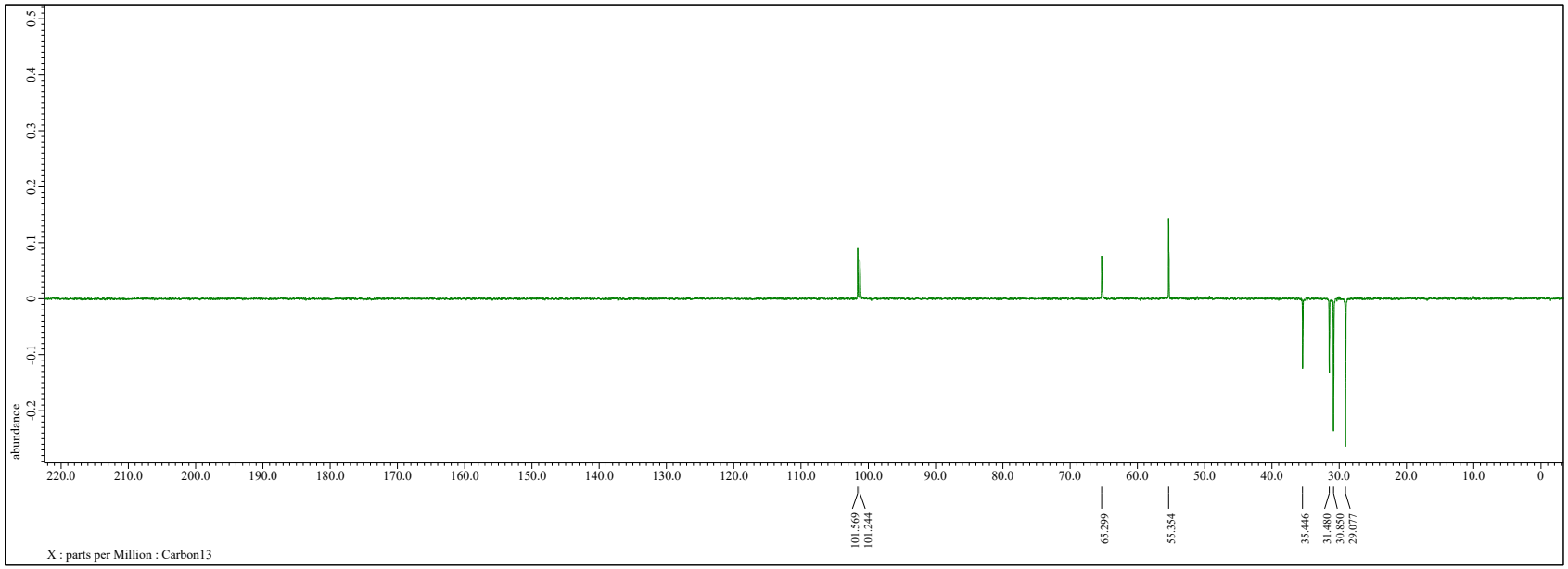


Figure S4. DEPT spectrum of **1** (Recorded in Acetone-*d6*)

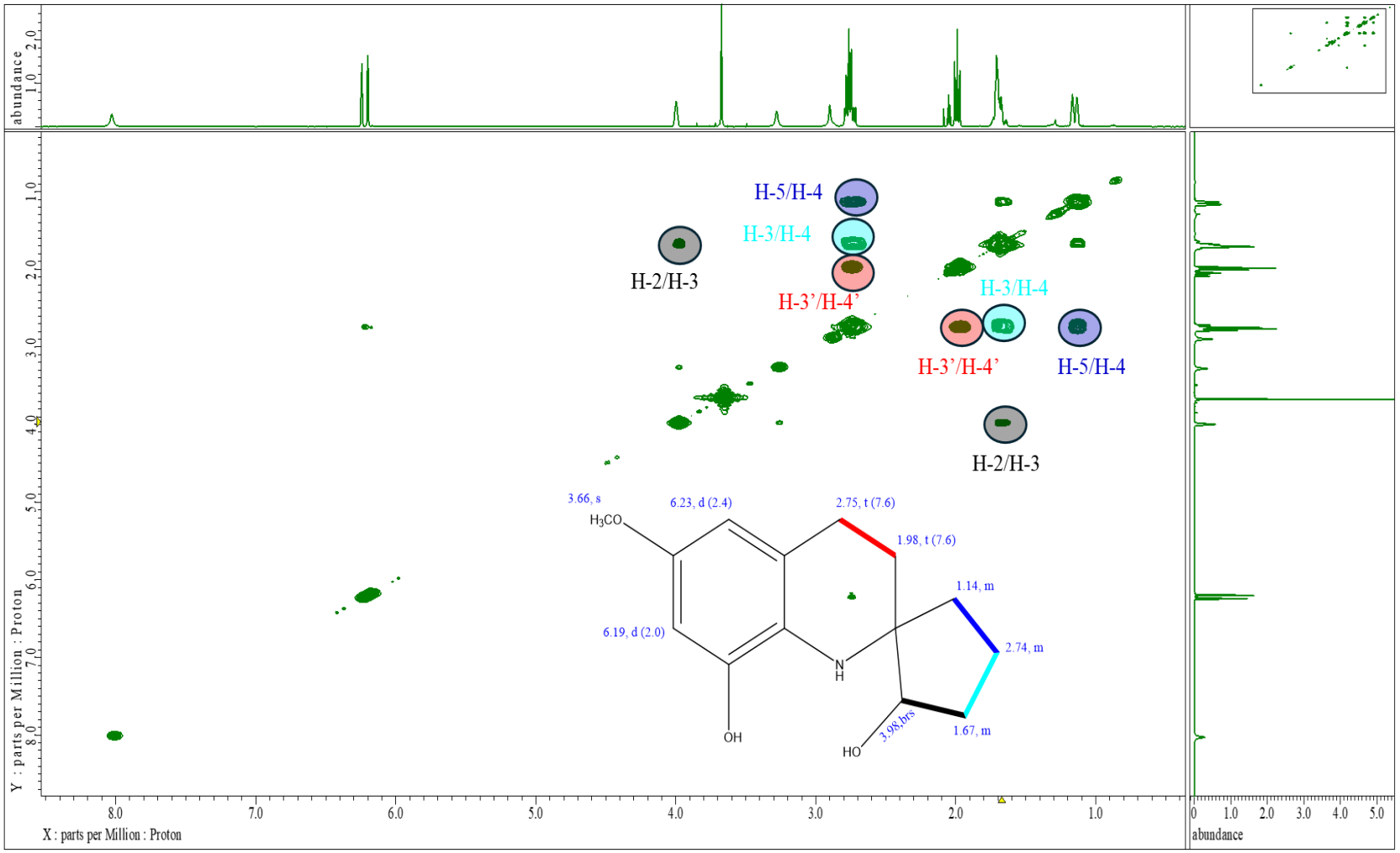


Figure S5. COSY spectrum of **1**

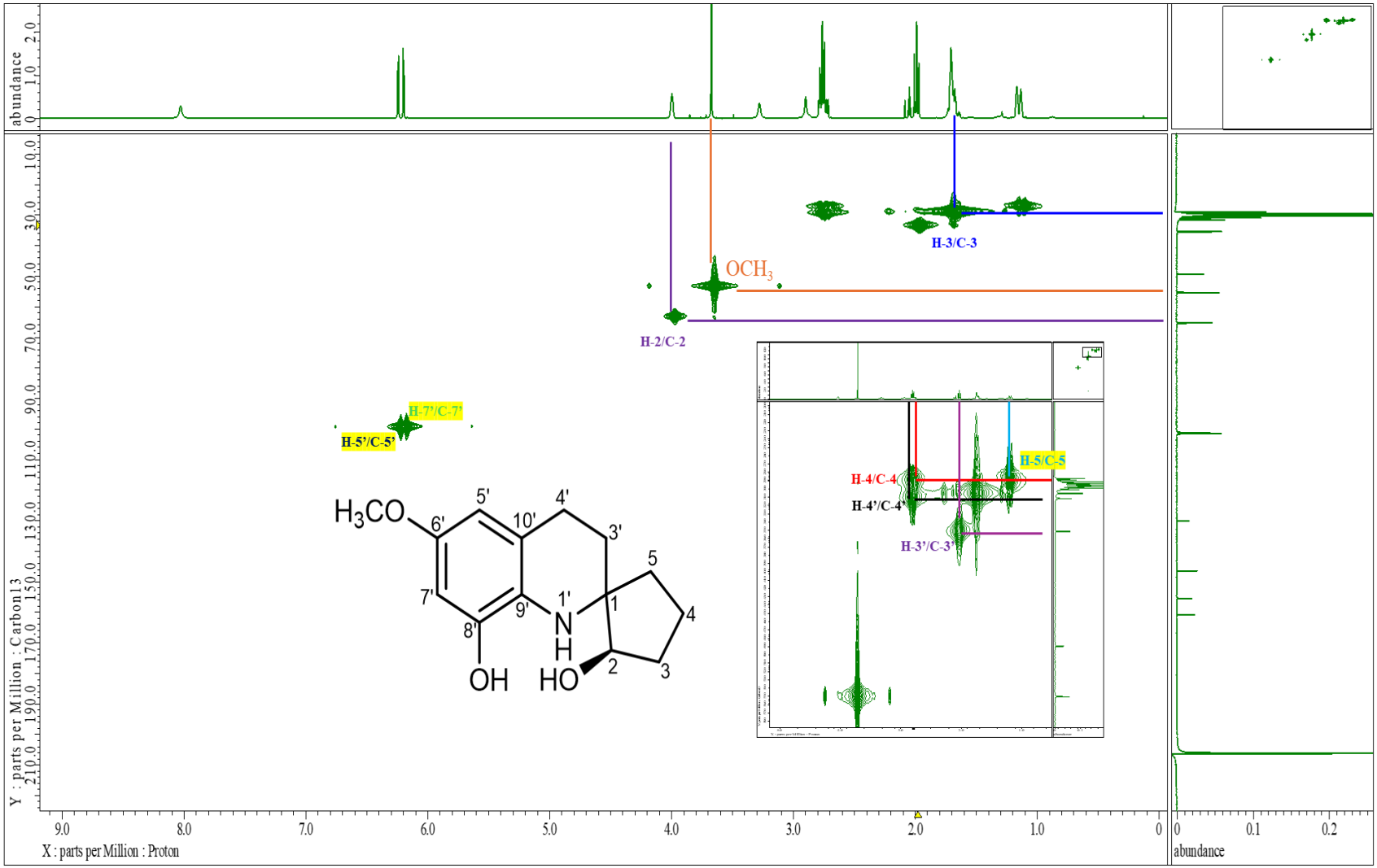


Figure S6. HMQC spectrum of **1**

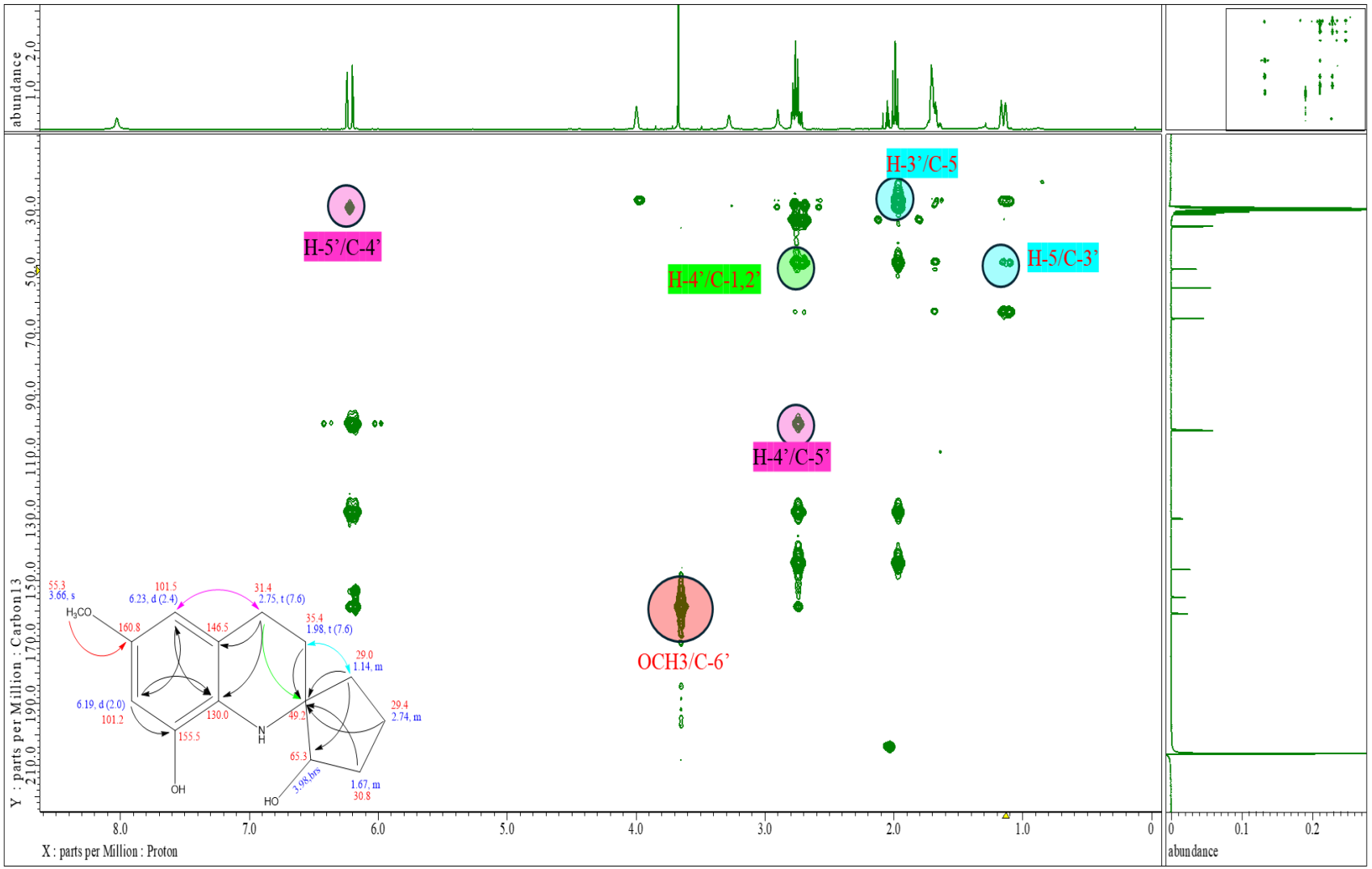


Figure S7. HMBC spectrum of **1**

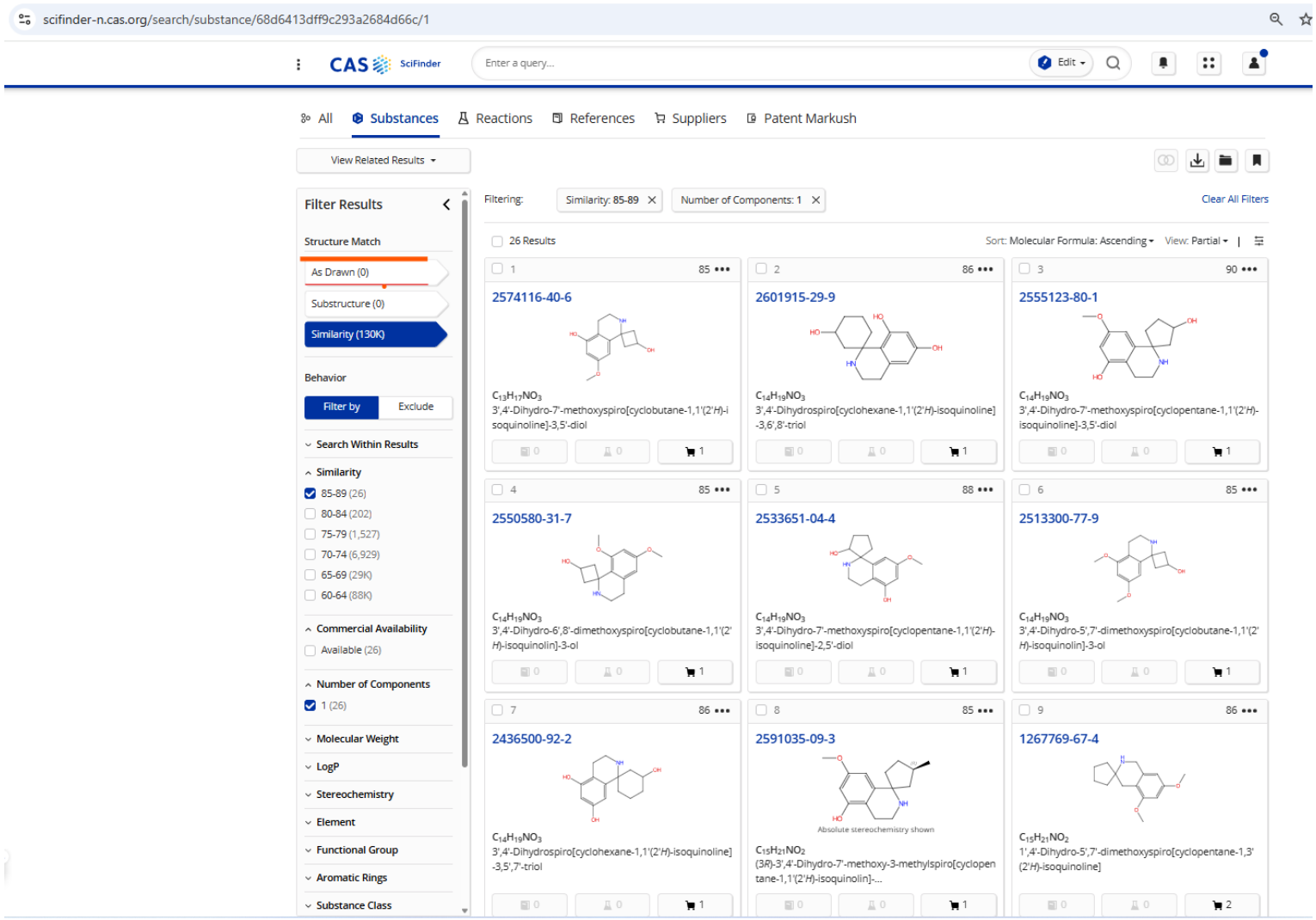
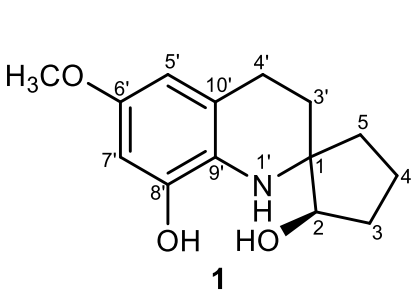


Figure S8. The research results for compound **1** were obtained from Scifider database

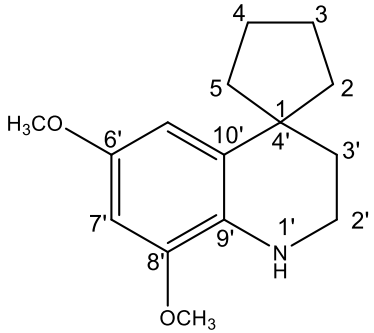
Table 1. The comparison ^{1}H and ^{13}C NMR spectroscopic data of **1** and **ref. compound**

Position	1[a]		ref. compound[b]	
	δ_{H} (J in Hz)	δ_{C}		
1	-	49.2	-	39.3
2	3.98 (1H, *brs*)	65.3	1.60 – 2.00 (m)	42.9
3	1.67 (2H, *m*)	30.8	1.60 – 2.00 (m)	25.3
4	2.73 (2H, *m*)	29.4	1.60 – 2.00 (m)	25.3
5	1.14 (2H, *m*)	29.0	1.60 – 2.00 (m)	42.9
1'	-	-	4.04 (1H, brs)	-
2'	-	-	3.25 (2H, *t*, 5.6)	36.0
3'	1.98 (2H, *t*, 7.6)	35.4	1.60 – 2.00 (m)	43.9
4'	2.75 (2H, *t*, 7.6)	31.4	-	-
5'	6.23 (1H, *d*, 2.2)	101.5	6.38 (1H, *d*, 2.4)	102.8
6'	-	160.8	-	151.4
7'	6.19 (1H, *d*, 2.2)	101.2	6.29 (1H, *d*, 2.4)	96.2
8'	-	155.5	-	147.0
9'	-	130.0	-	128.5
10'	-	146.5	-	130.7
OCH_3	3.66 (3H, *s*)	55.3	3.75 (3H, *s*)	55.8
OCH_3	-	-	3.80 (3H, *s*)	55.4

a: recorded in acetone-*d6*; b: recorded in $CDCl_3$; ref.compound: (6',8'-Dimethoxy-2',3'-dihydro-1'H-spiro[cyclopentane-1,4-quinolin] [1]



1



ref. compound

2. Spectroscopic data for compound 2

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{21}H_{30}O_2$	315.2319	315.2319	- 0.14 / - 0.04

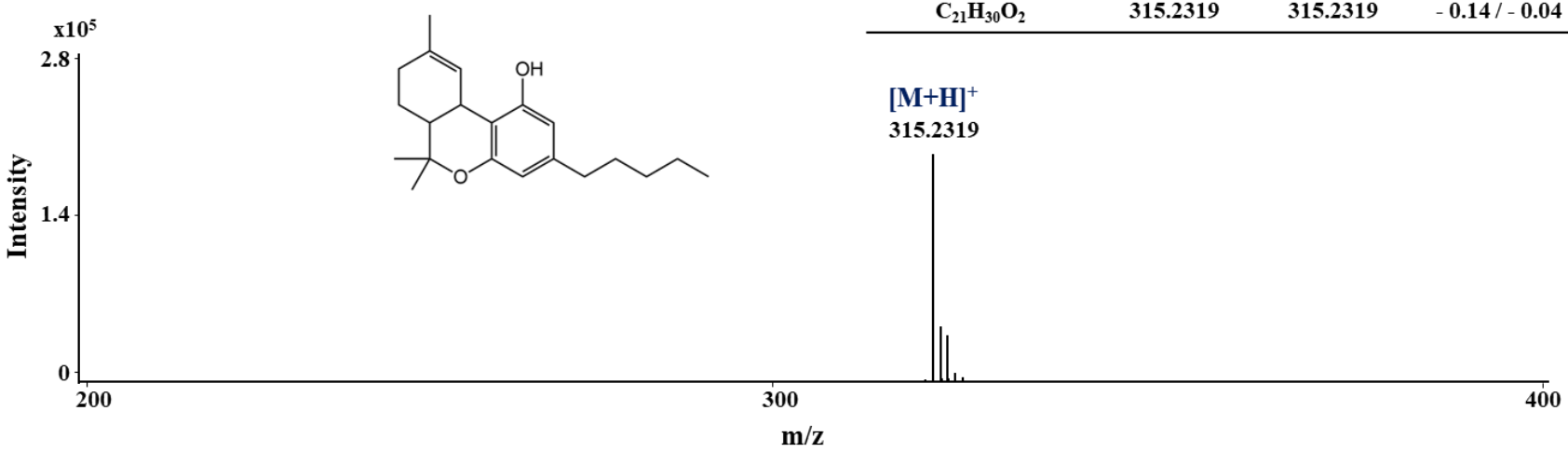


Figure S9. MS spectrum of **2**

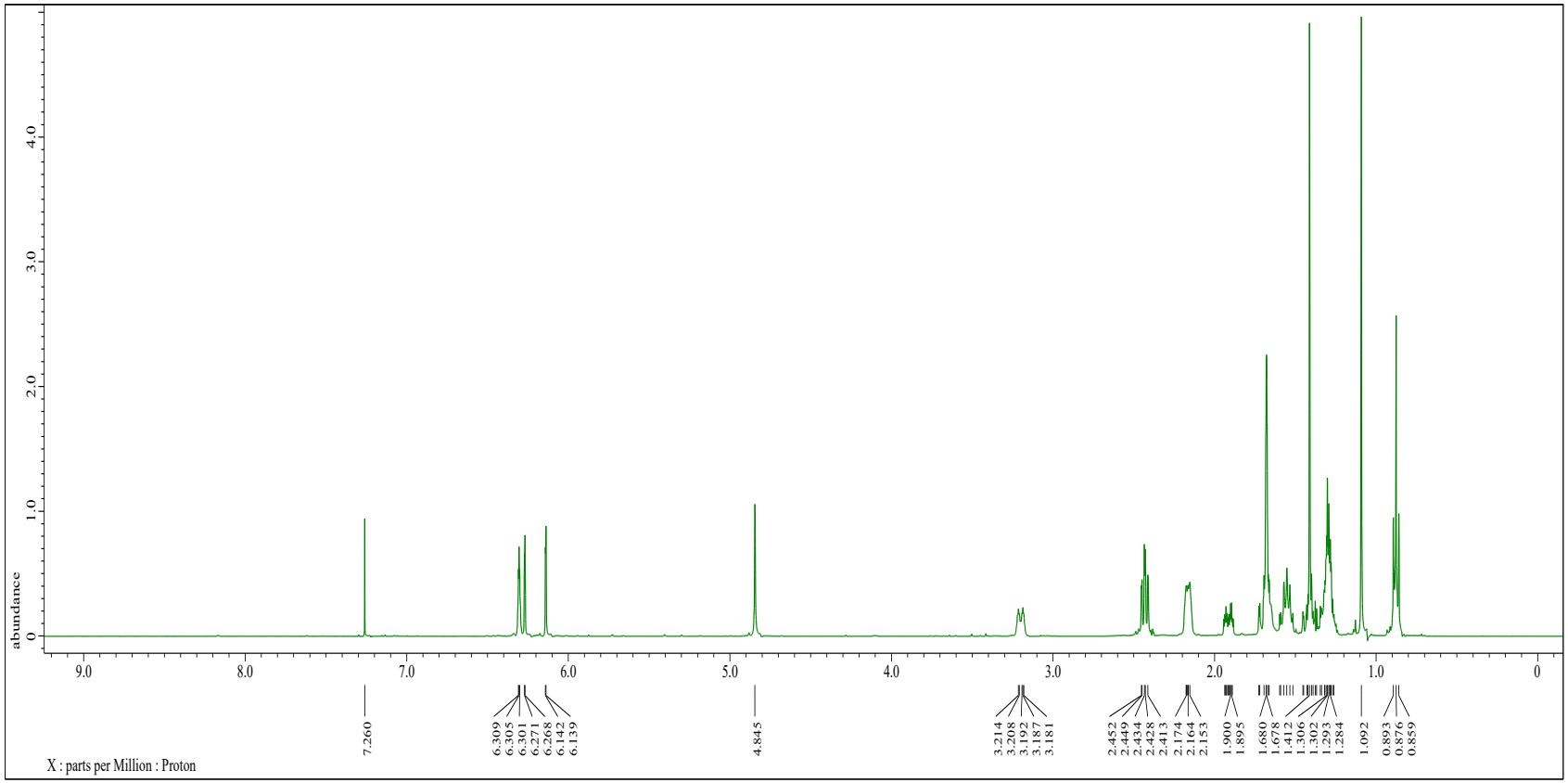


Figure S10. ^{1}H NMR spectrum of **2** (Recorded in $CDCl_3$)

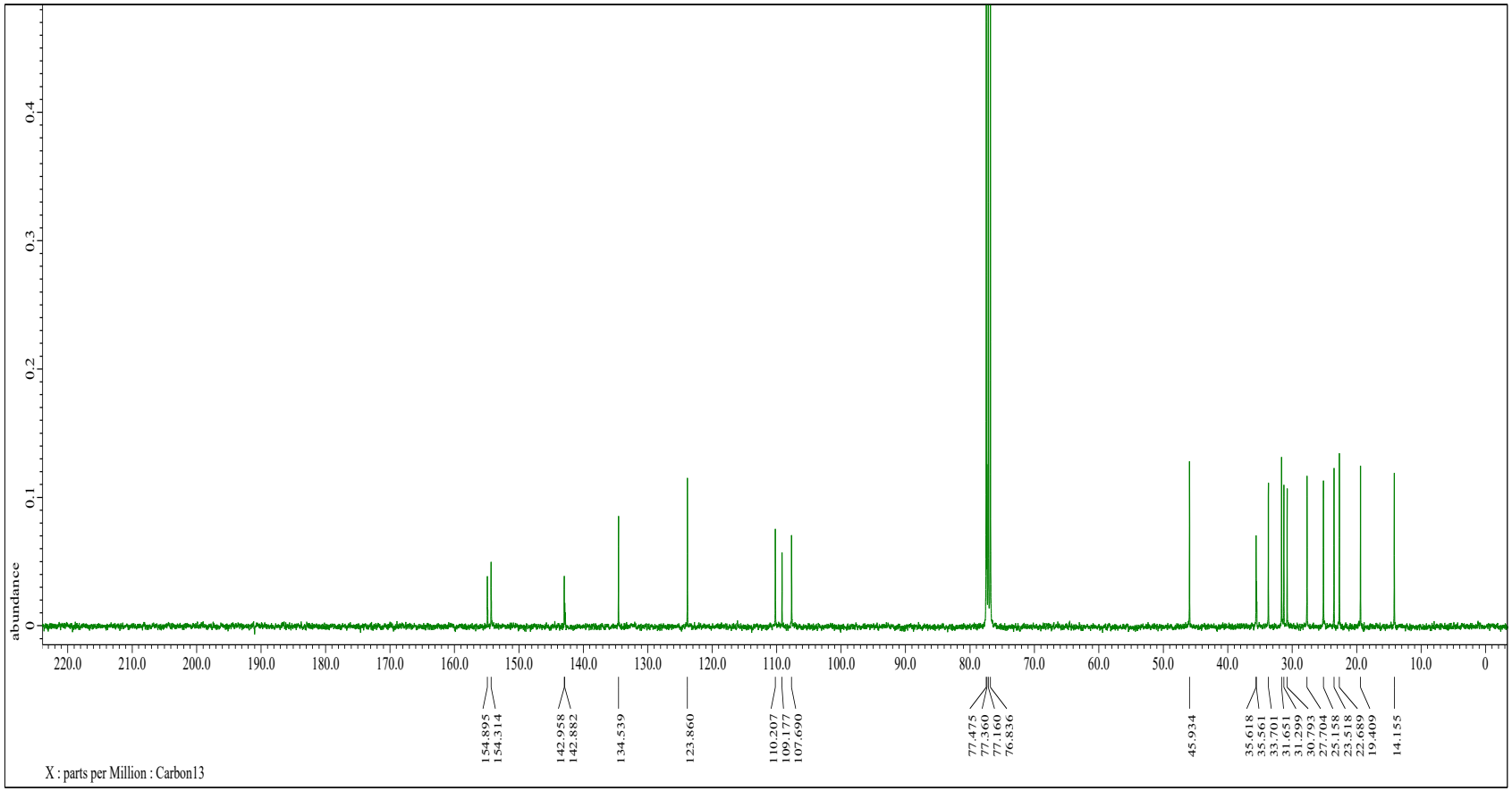


Figure S11. ^{13}C NMR spectrum of **2** (Recorded in $CDCl_3$)

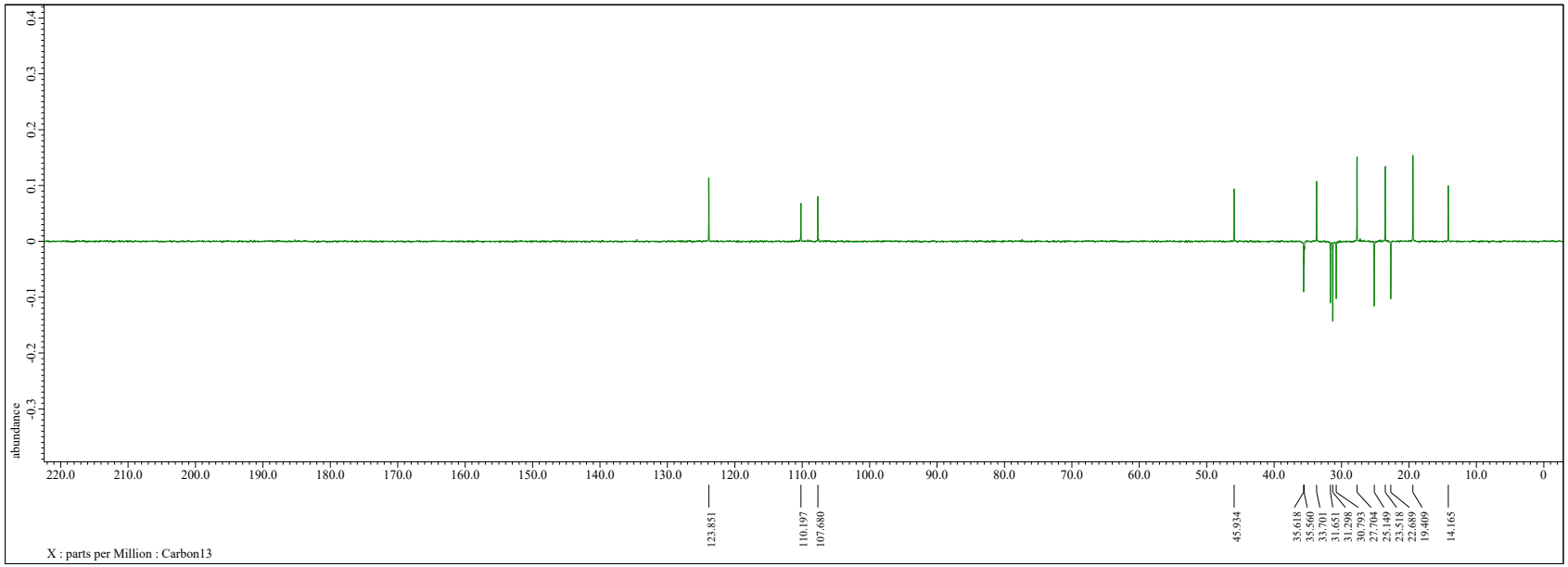


Figure S12. DEPT spectrum of **2** (Recorded in $CDCl_3$)

3. Spectroscopic data for compound 3

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{22}H_{32}O_4$	361.2373	361.2367	1.76 / 0.64

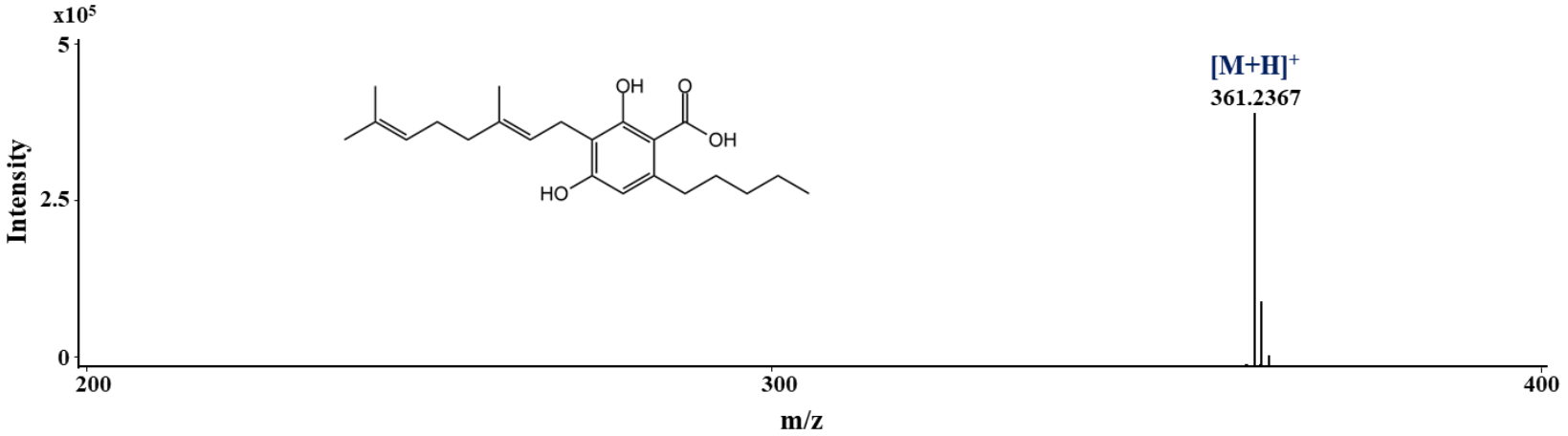


Figure S13. MS spectrum of **3**

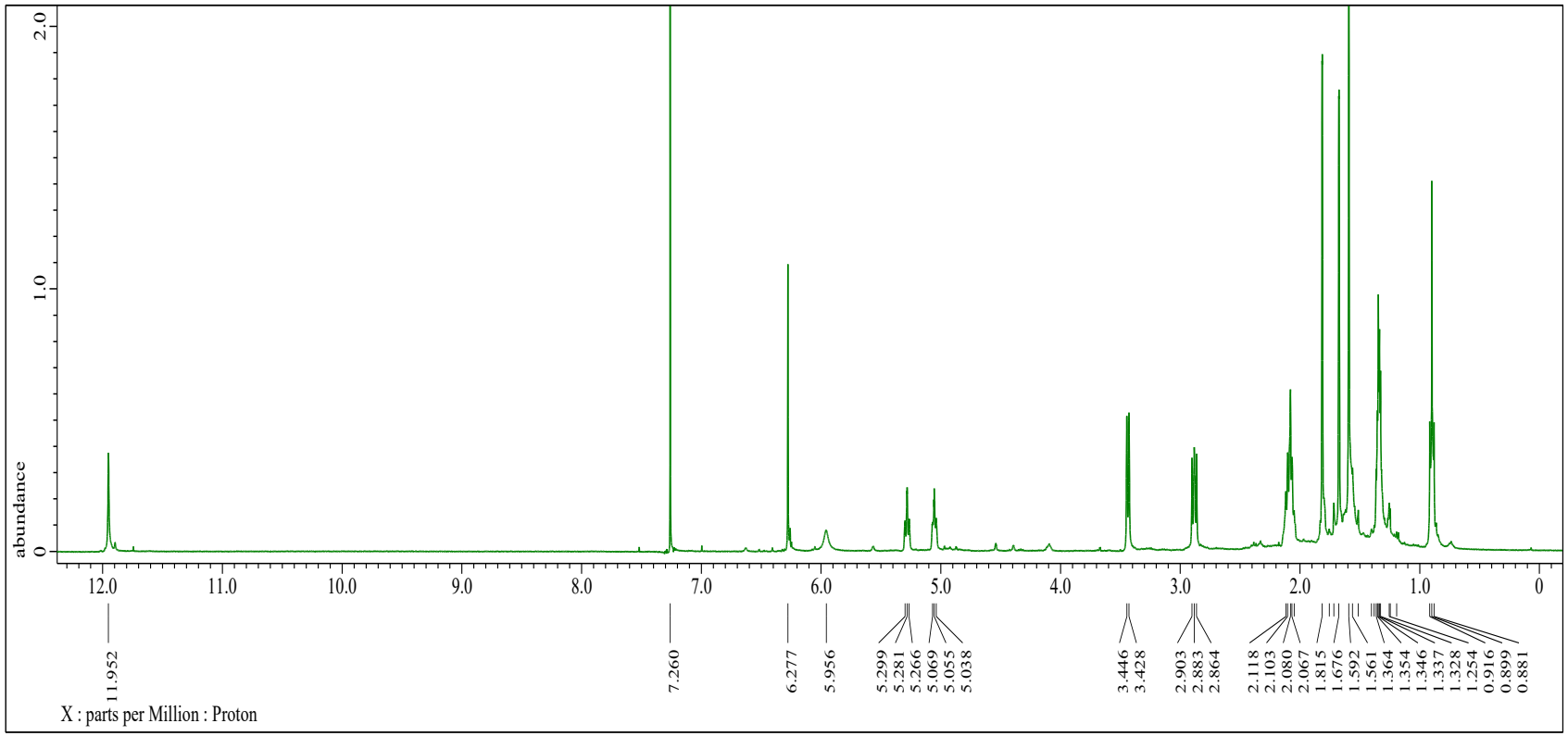


Figure S14. ^{1}H NMR spectrum of **3** (Recorded in $CDCl_3$)

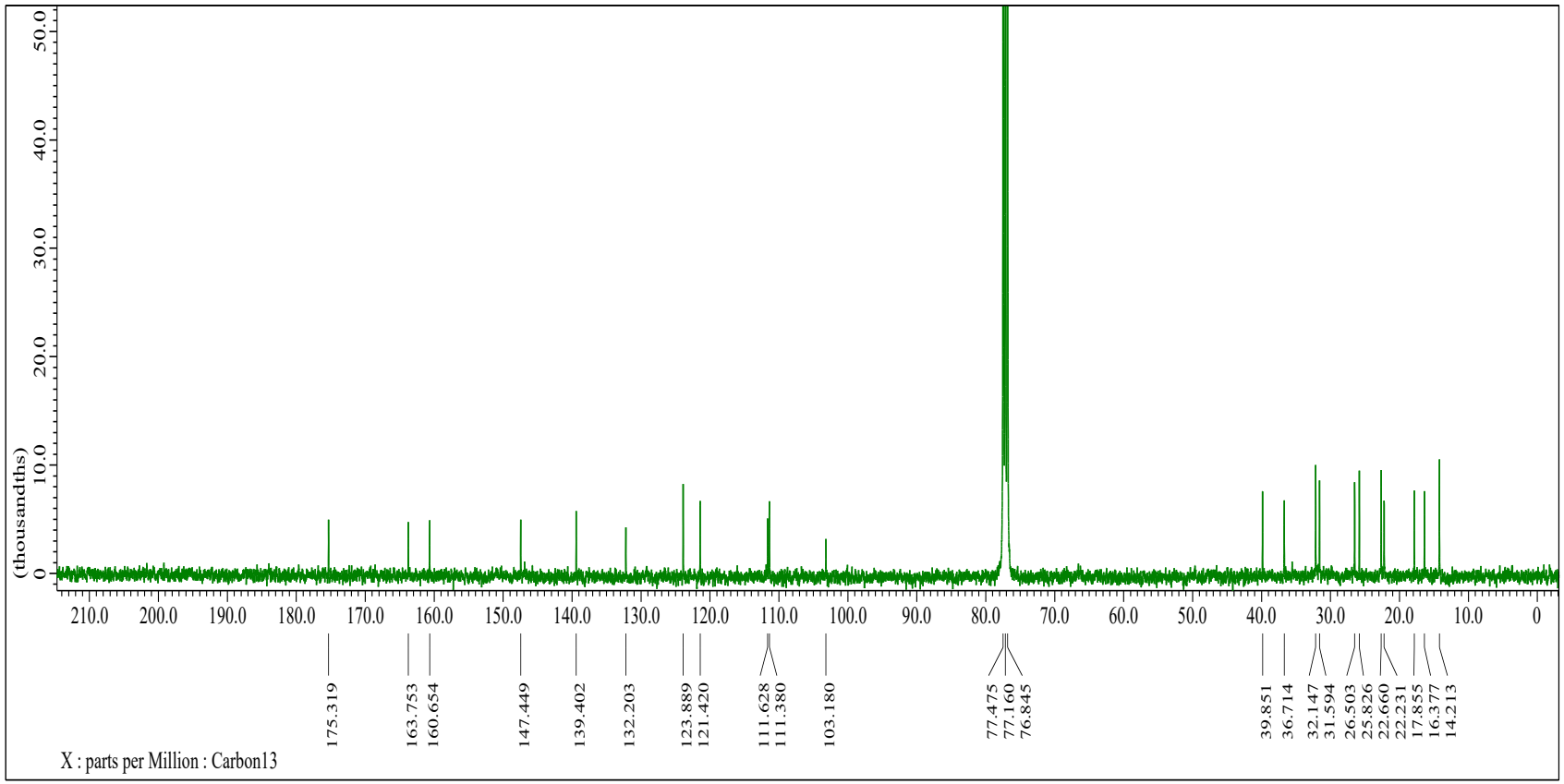


Figure S15. ^{13}C NMR spectrum of **3** (Recorded in $CDCl_3$)

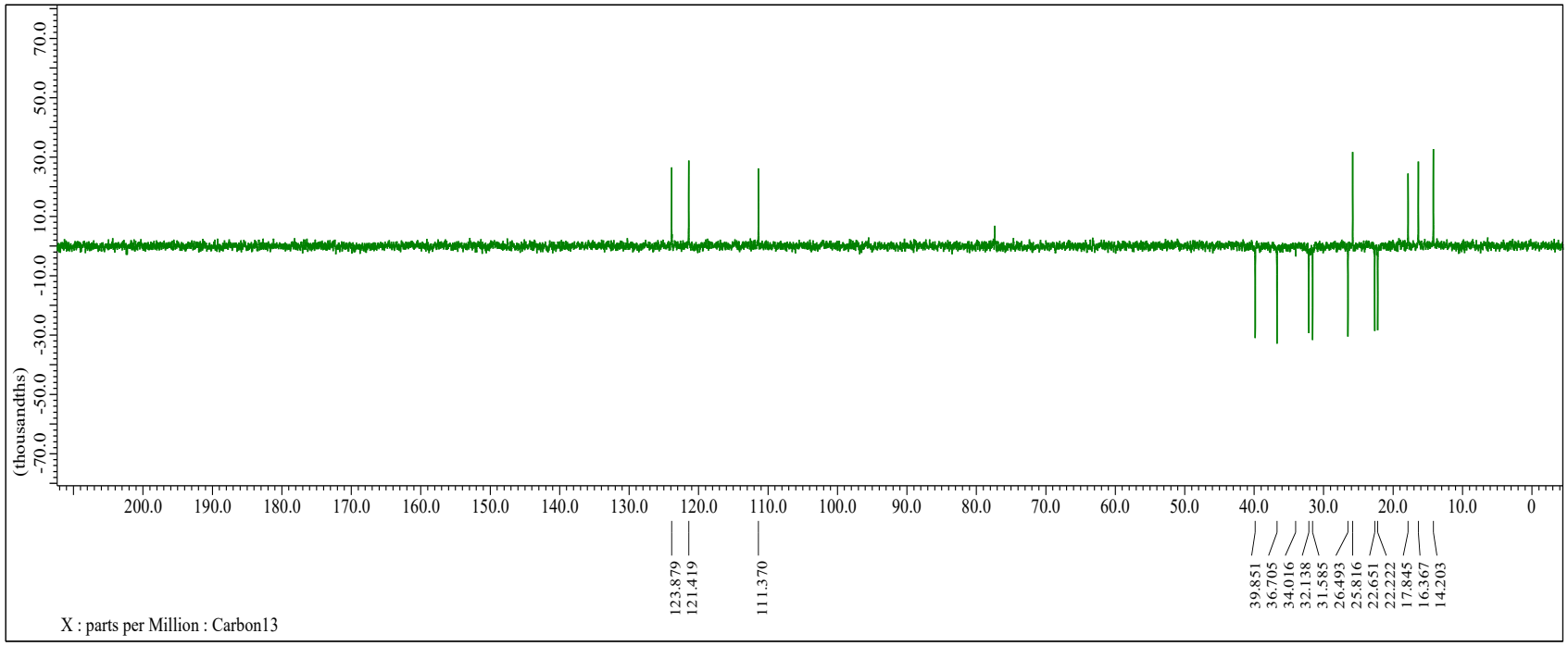


Figure S16. DEPT spectrum of **3**

4. Spectroscopic data for compound 4

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{21}H_{30}O_2$	315.2319	315.2316	0.81 / 0.26

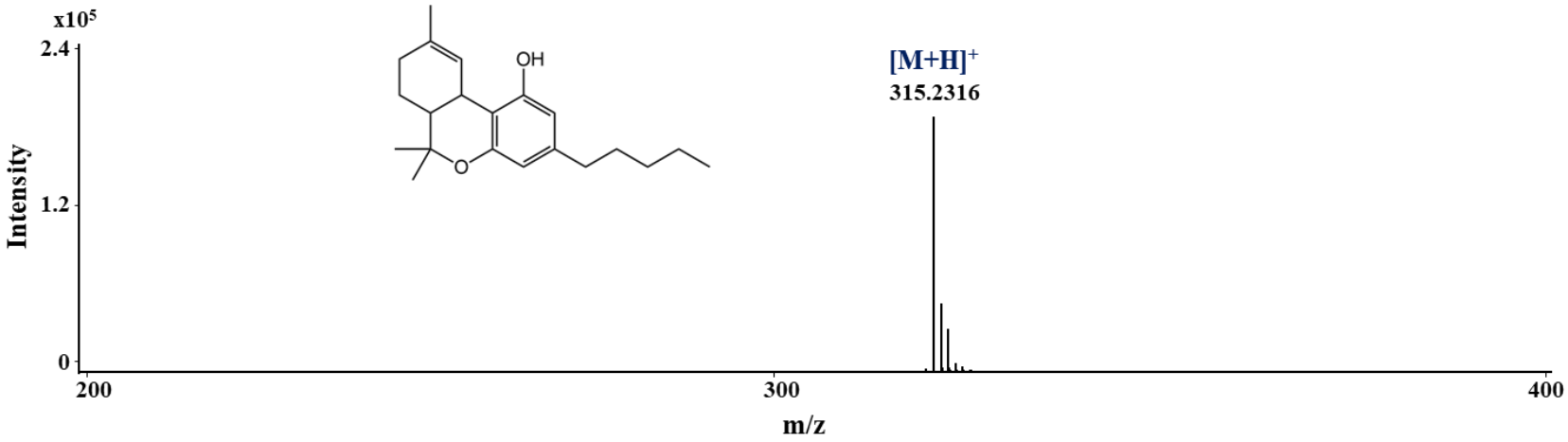


Figure S17. MS spectrum of **4**

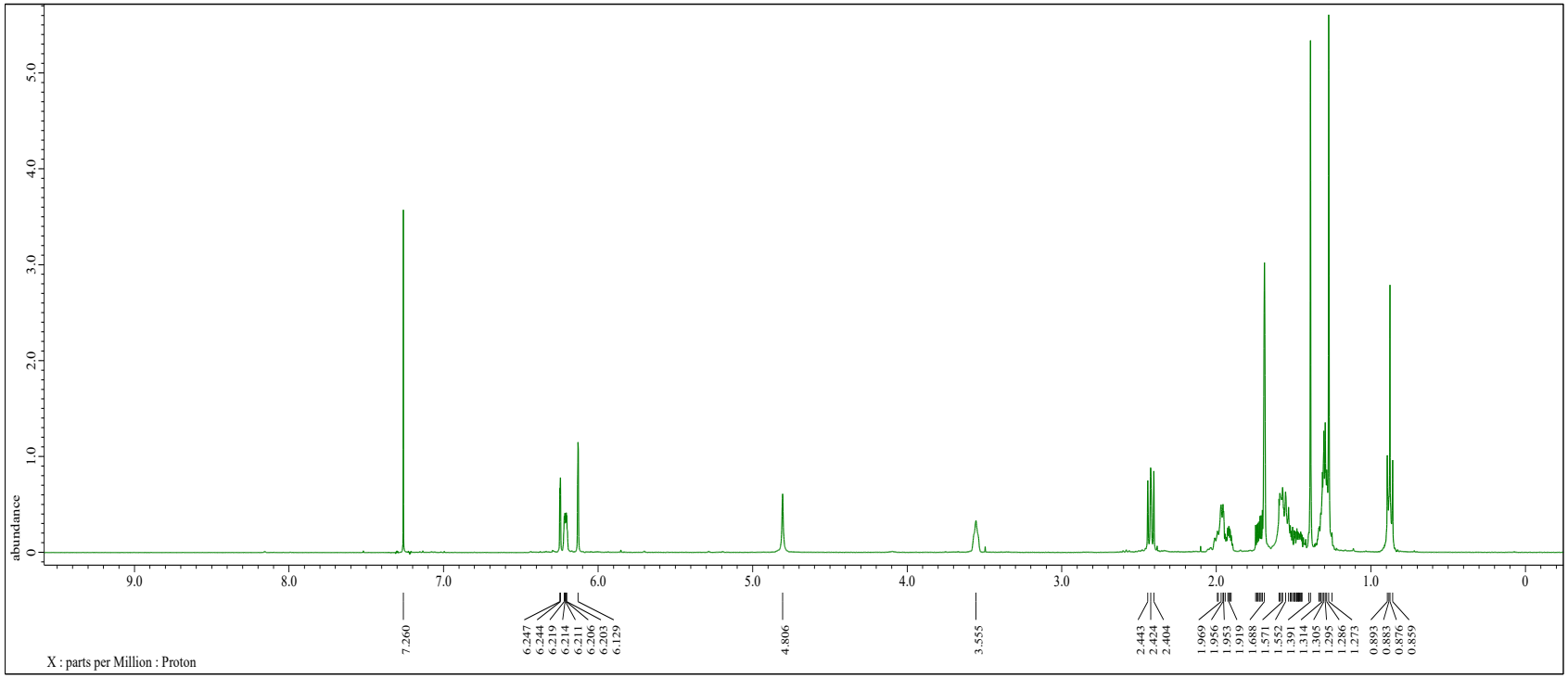


Figure S18. ^{1}H NMR spectrum of **4** (Recorded in $CDCl_3$)

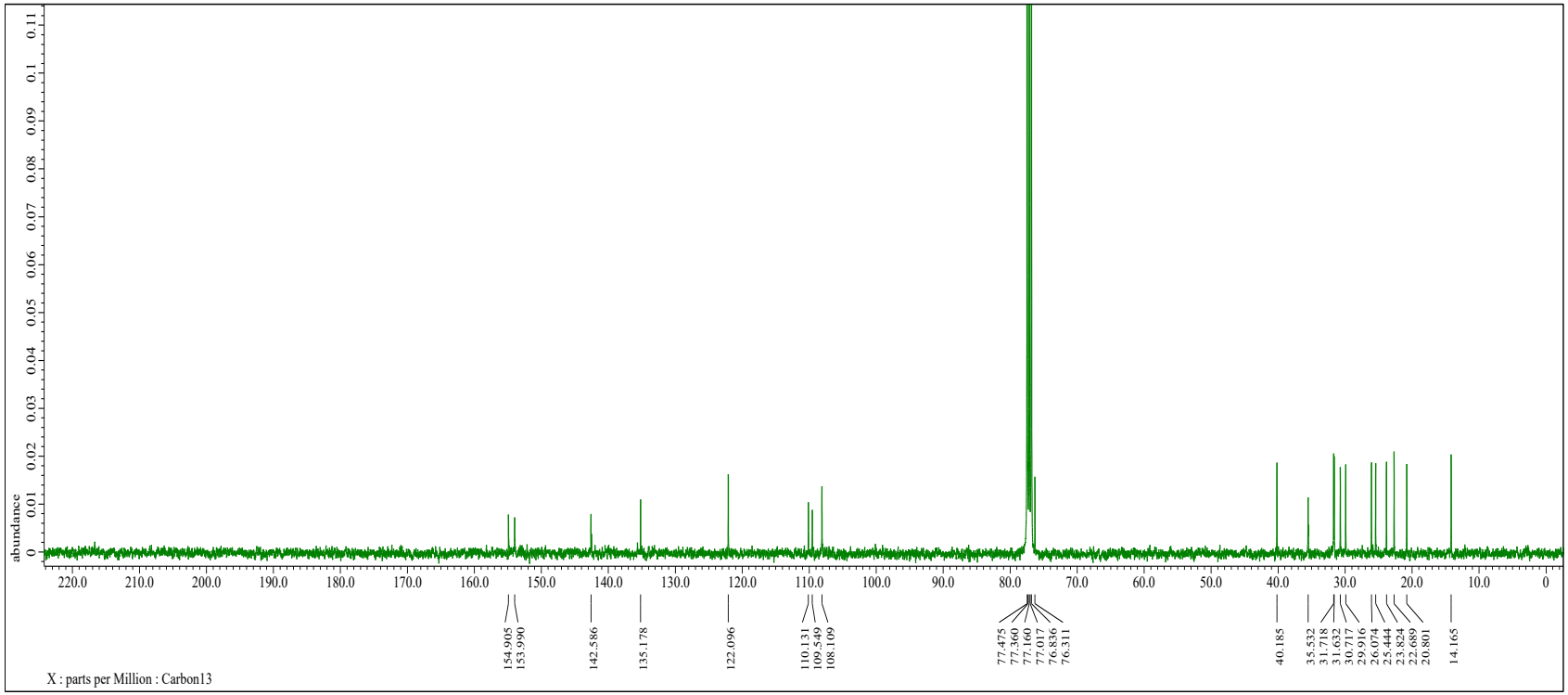


Figure S19. ^{13}C NMR spectrum of **4** (Recorded in $CDCl_3$)

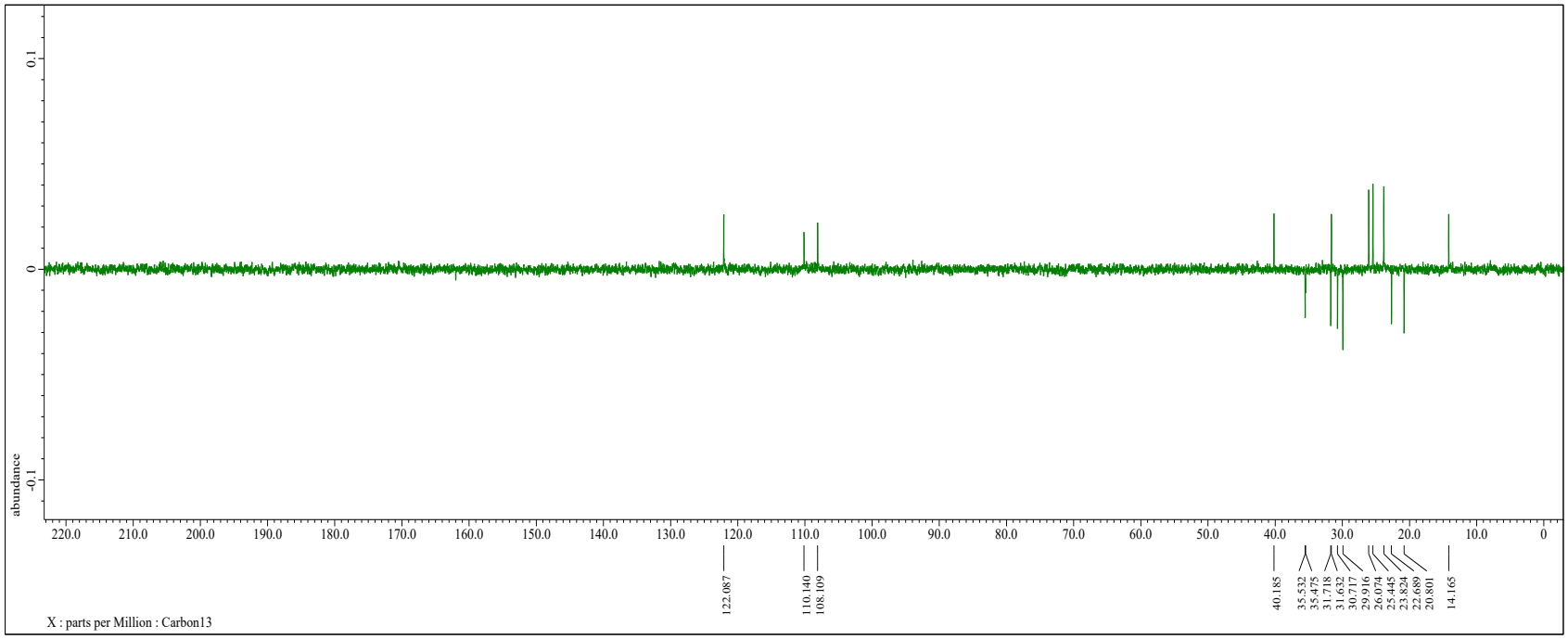


Figure S20. DEPT spectrum of **4**

5. Spectroscopic data for compound 5

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{15}H_{26}O$	223.2056	223.2053	1.53 / 0.34

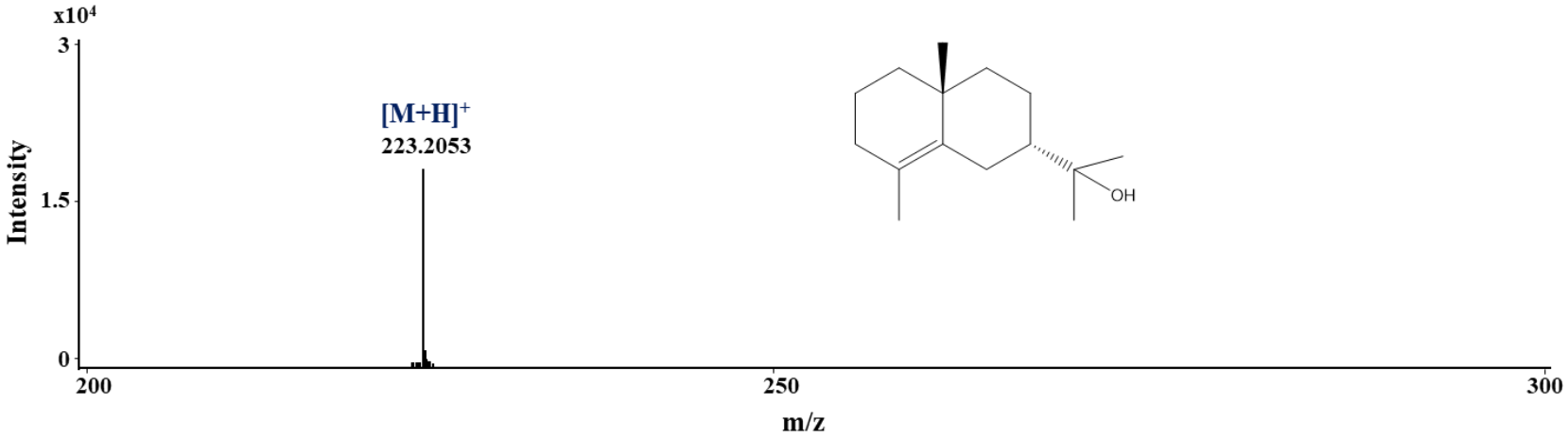


Figure S21. MS spectrum of **5**

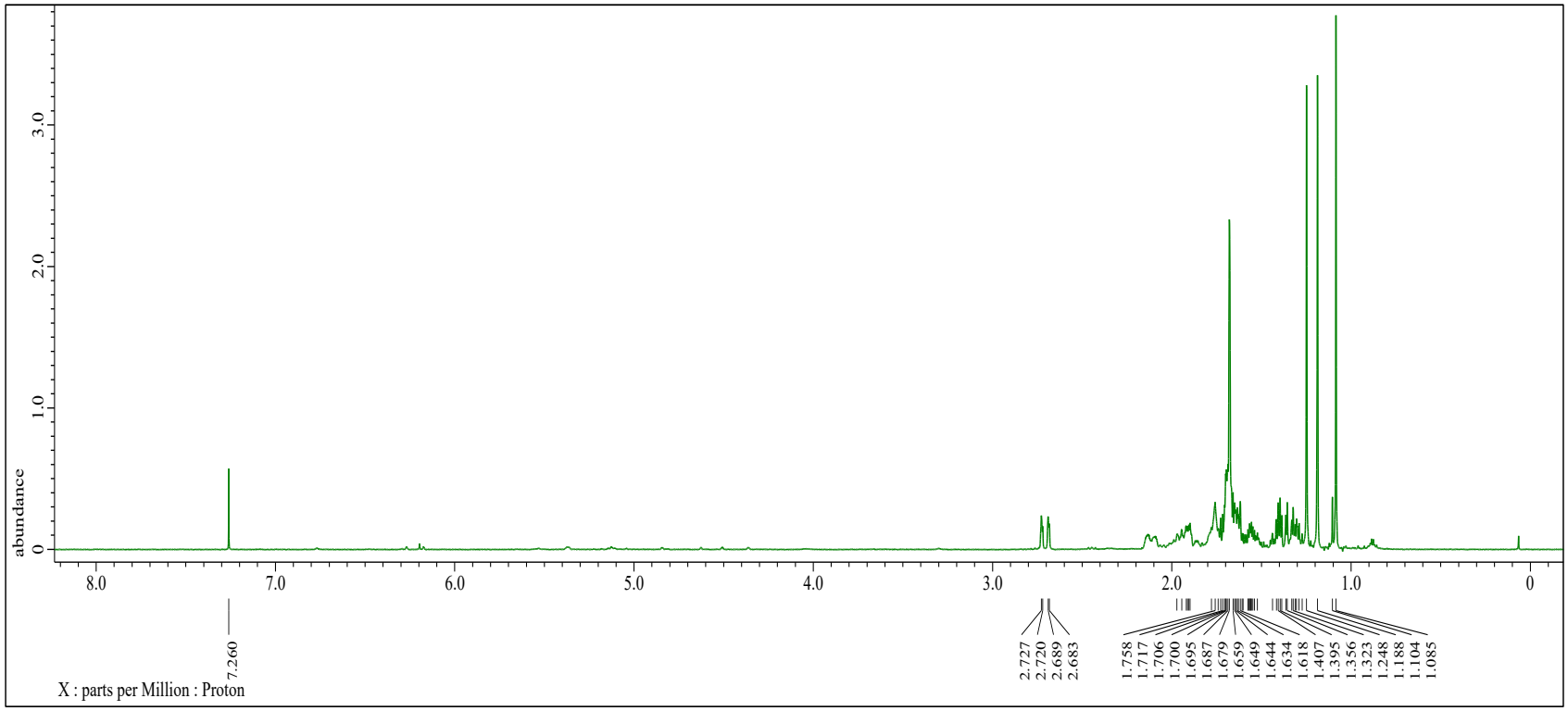


Figure S22. ^{1}H NMR spectrum of **5** (Recorded in $CDCl_3$)

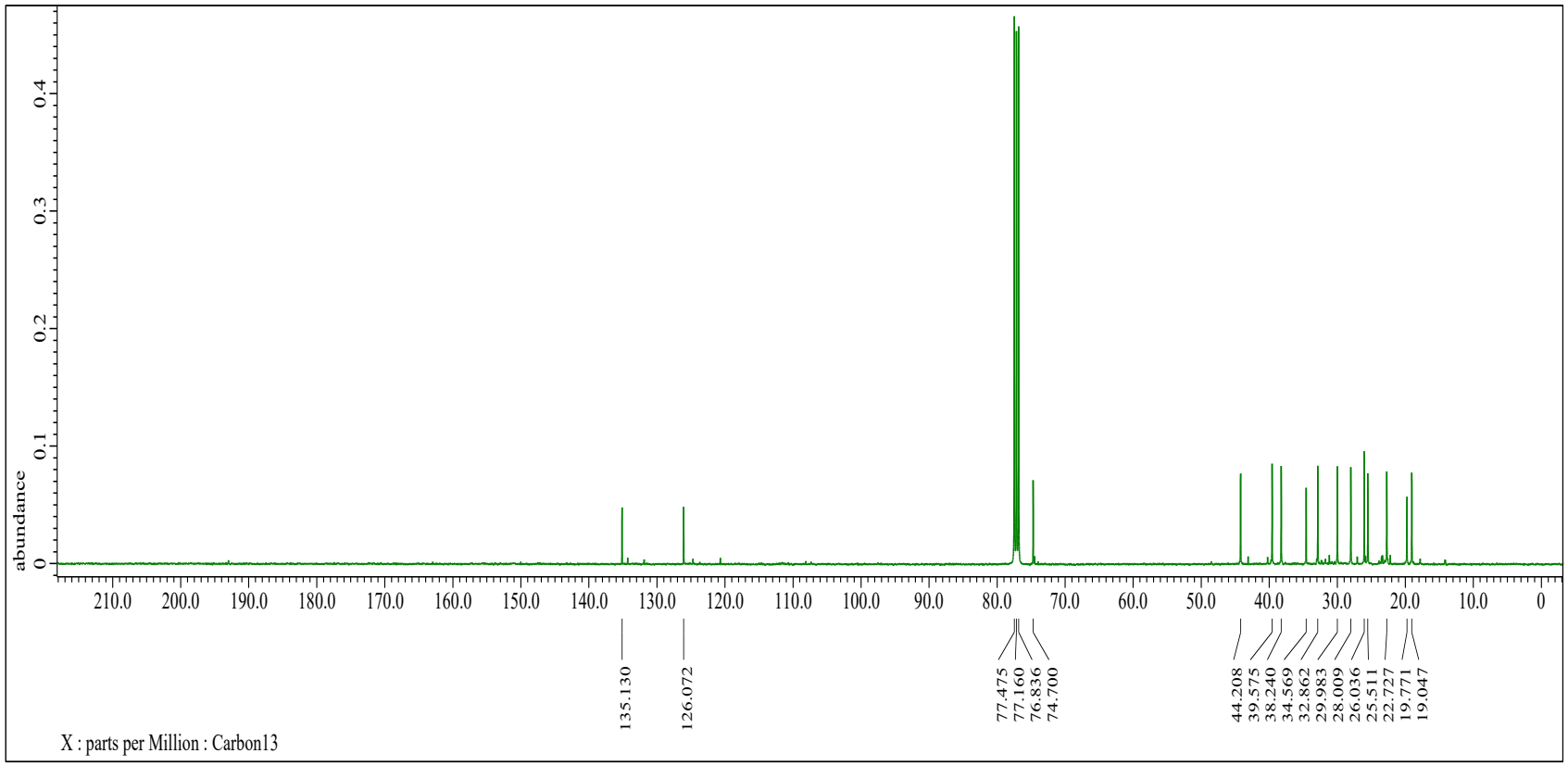


Figure S23. ^{13}C NMR spectrum of **5** (Recorded in $CDCl_3$)

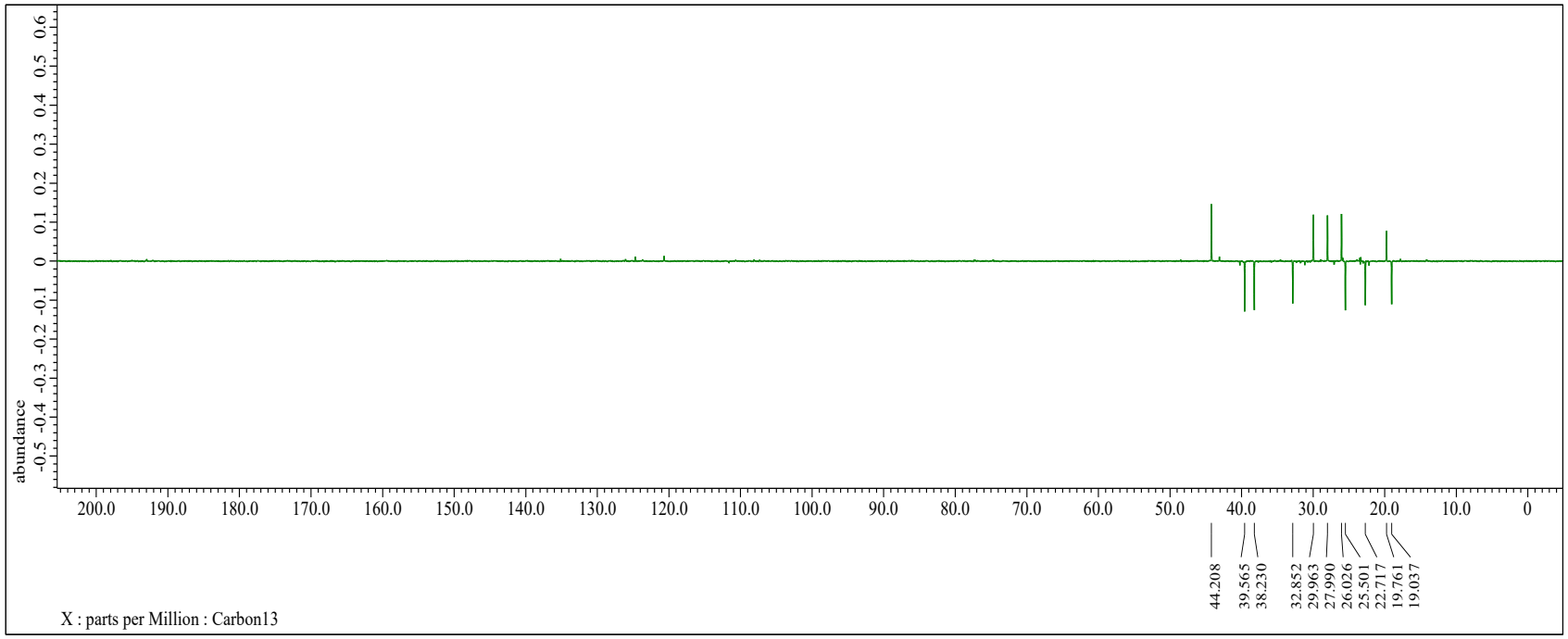


Figure S24. DEPT spectrum of **5** (Recorded in $CDCl_3$)

6. Spectroscopic data for compound 6

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{15}H_{26}O$	223.2056	223.2044	5.56 / 1.24

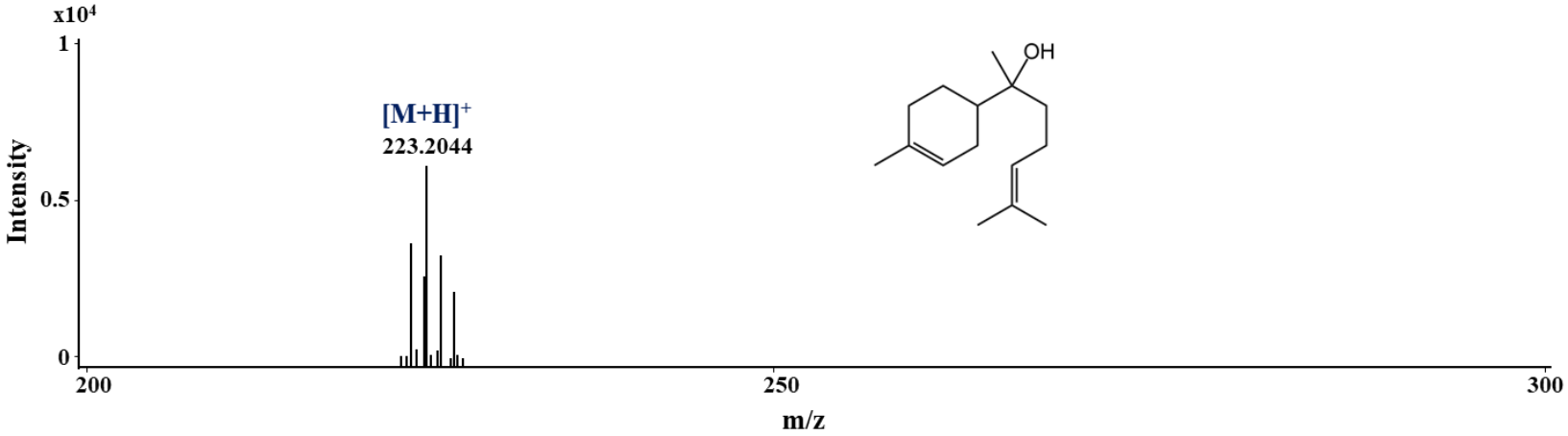


Figure S25. MS spectrum of **6**

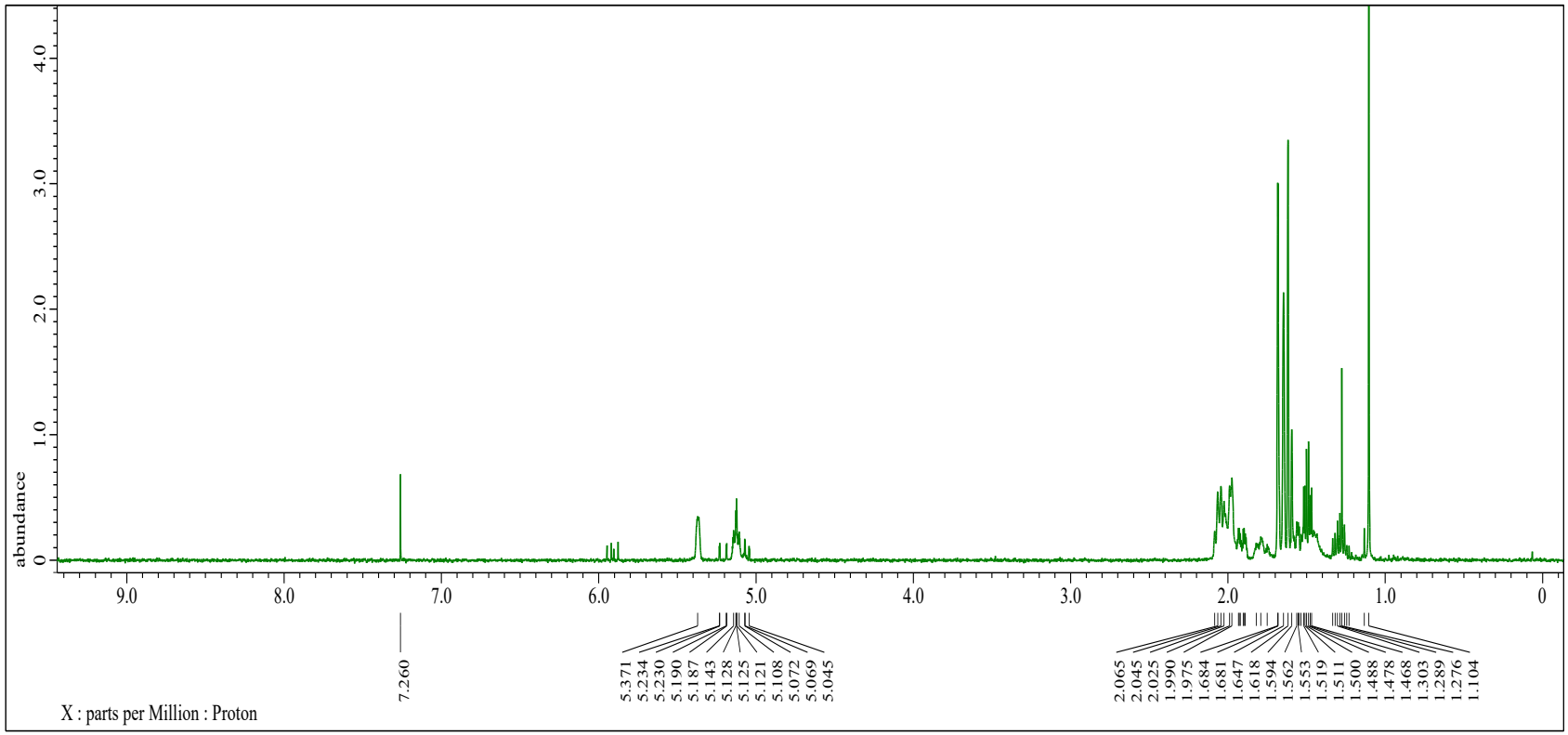


Figure S26. ^{1}H NMR spectrum of **6** (Recorded in $CDCl_3$)

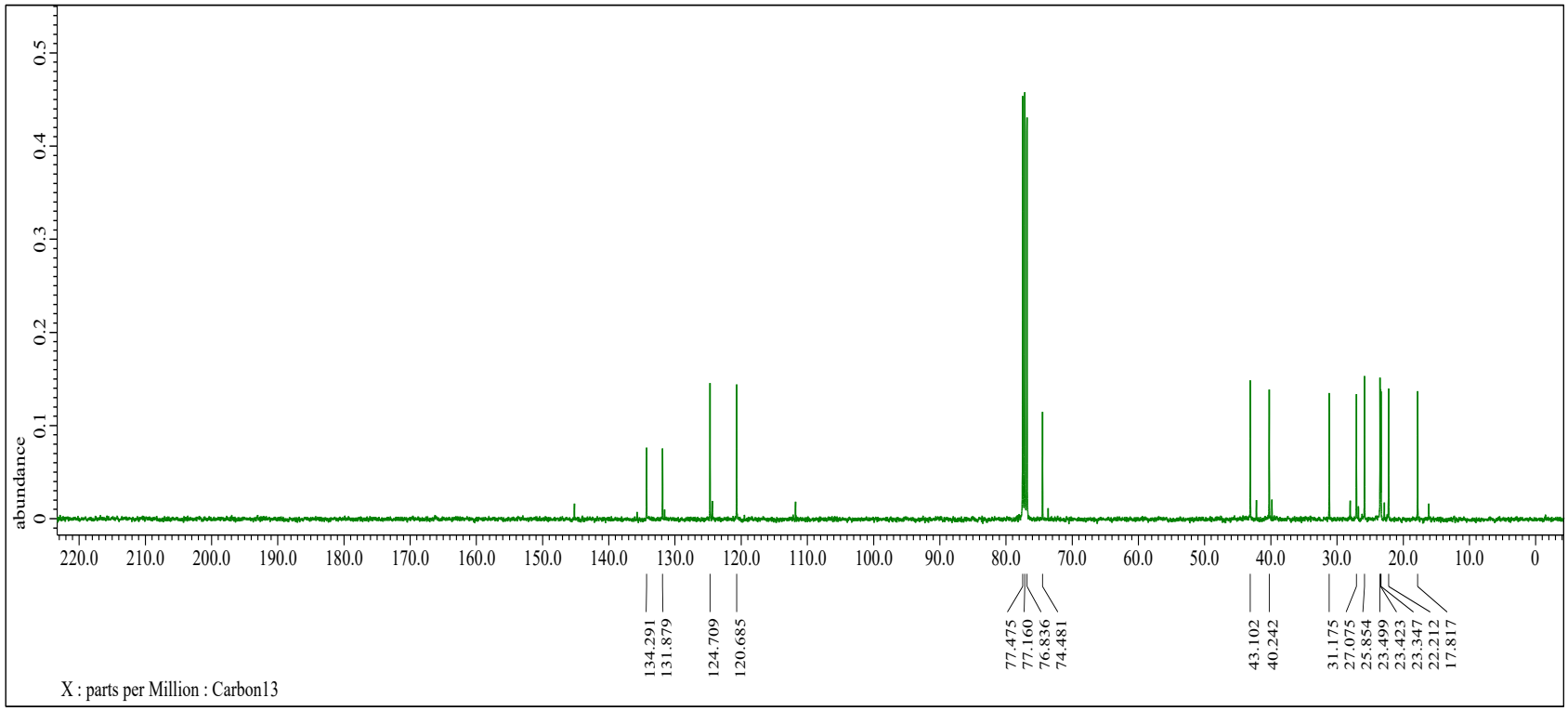


Figure S27. ^{13}C NMR spectrum of **6**

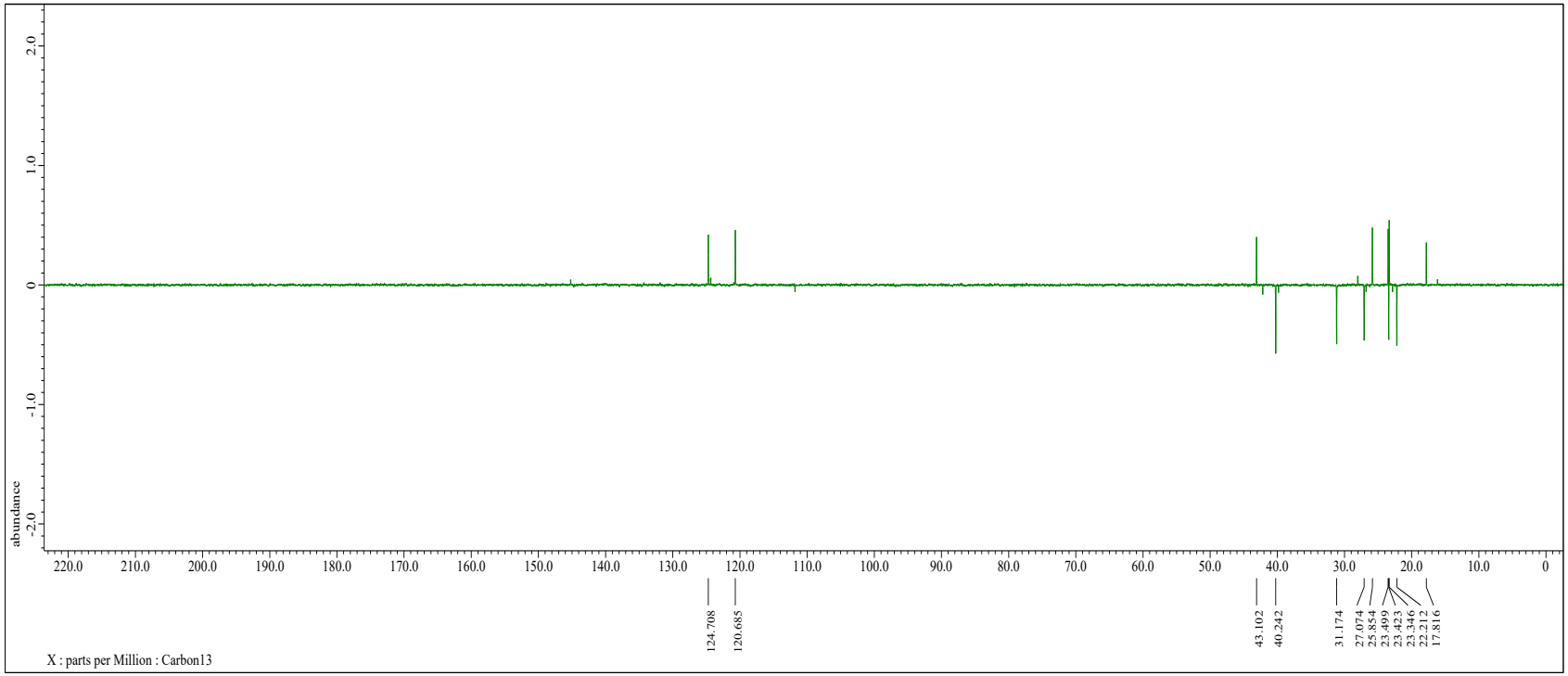


Figure S28. DEPT spectrum of **6**

7. Spectroscopic data for compound 7

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{15}H_{26}O$	223.2056	223.2062	-2.5 / -0.56

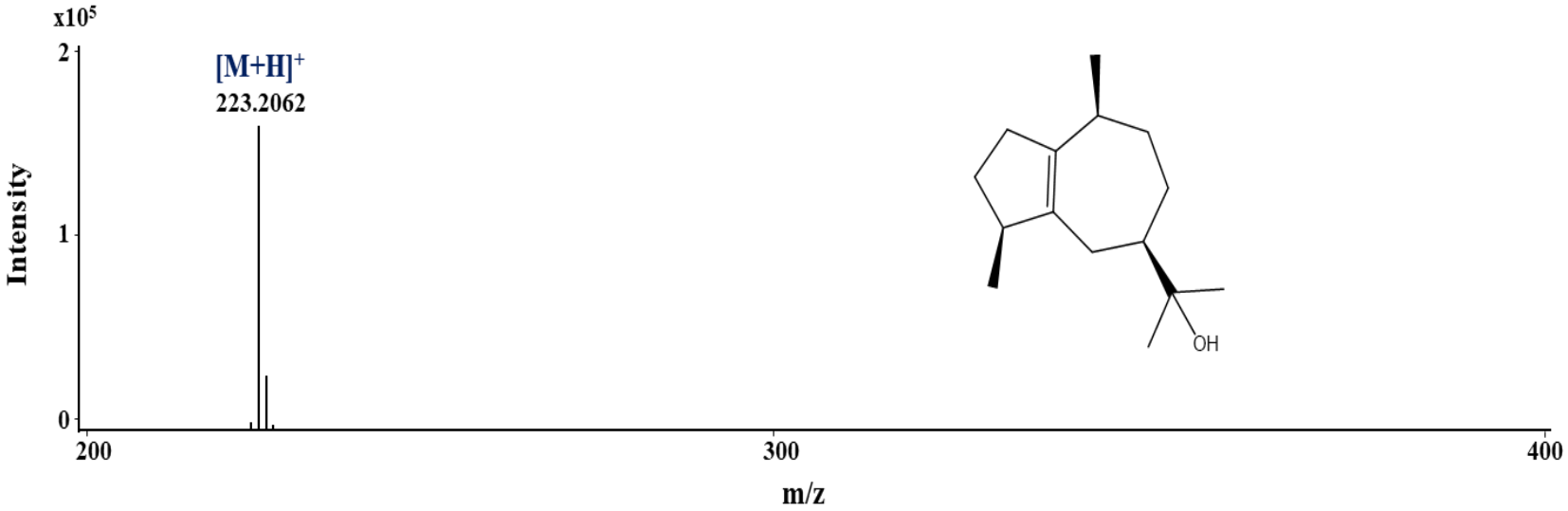


Figure S29. MS spectrum of **7**

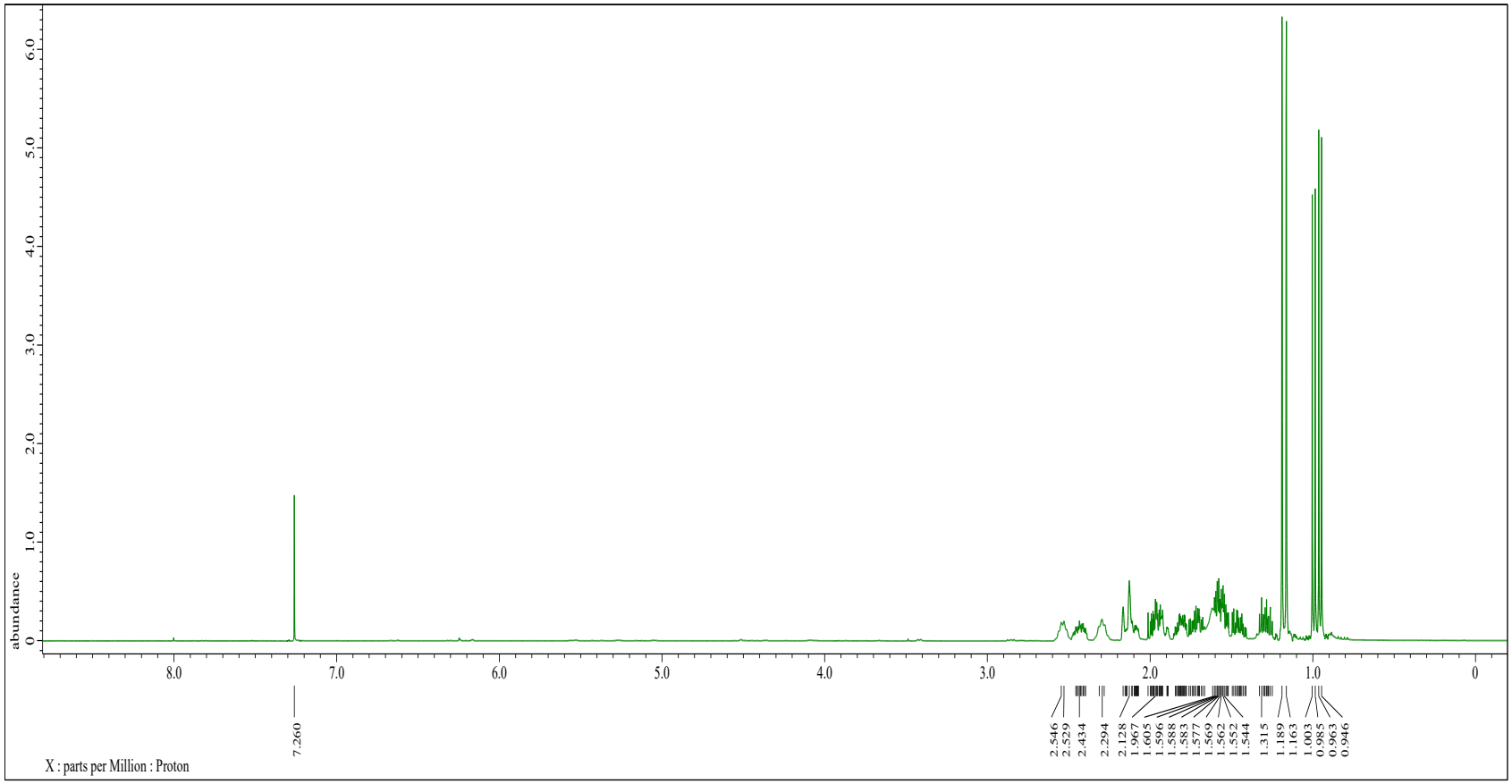


Figure S30. ^{1}H NMR spectrum of **7** (Recorded in $CDCl_3$)

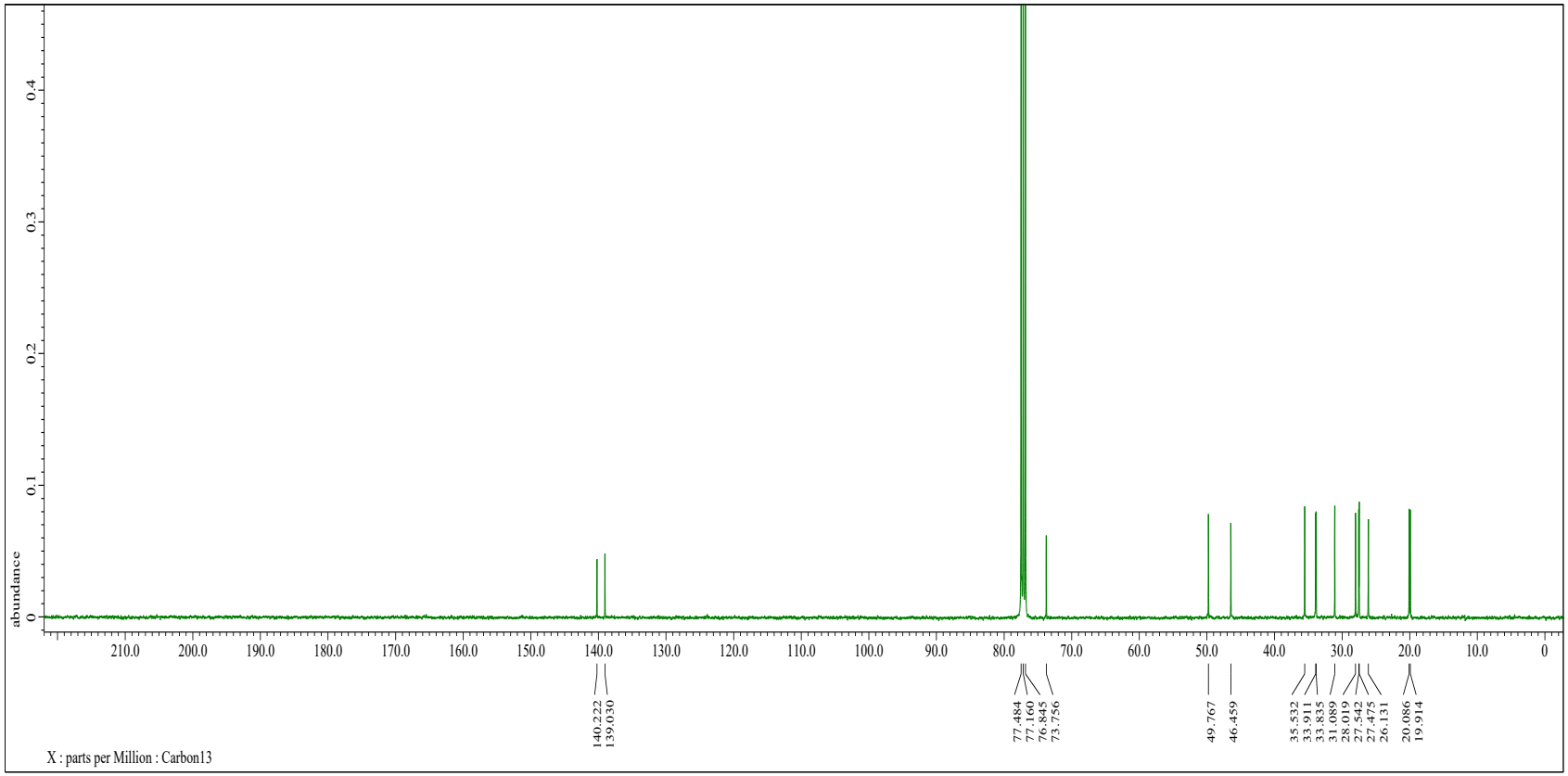


Figure S31. ^{13}C NMR spectrum of **7** (Recorded in $CDCl_3$)

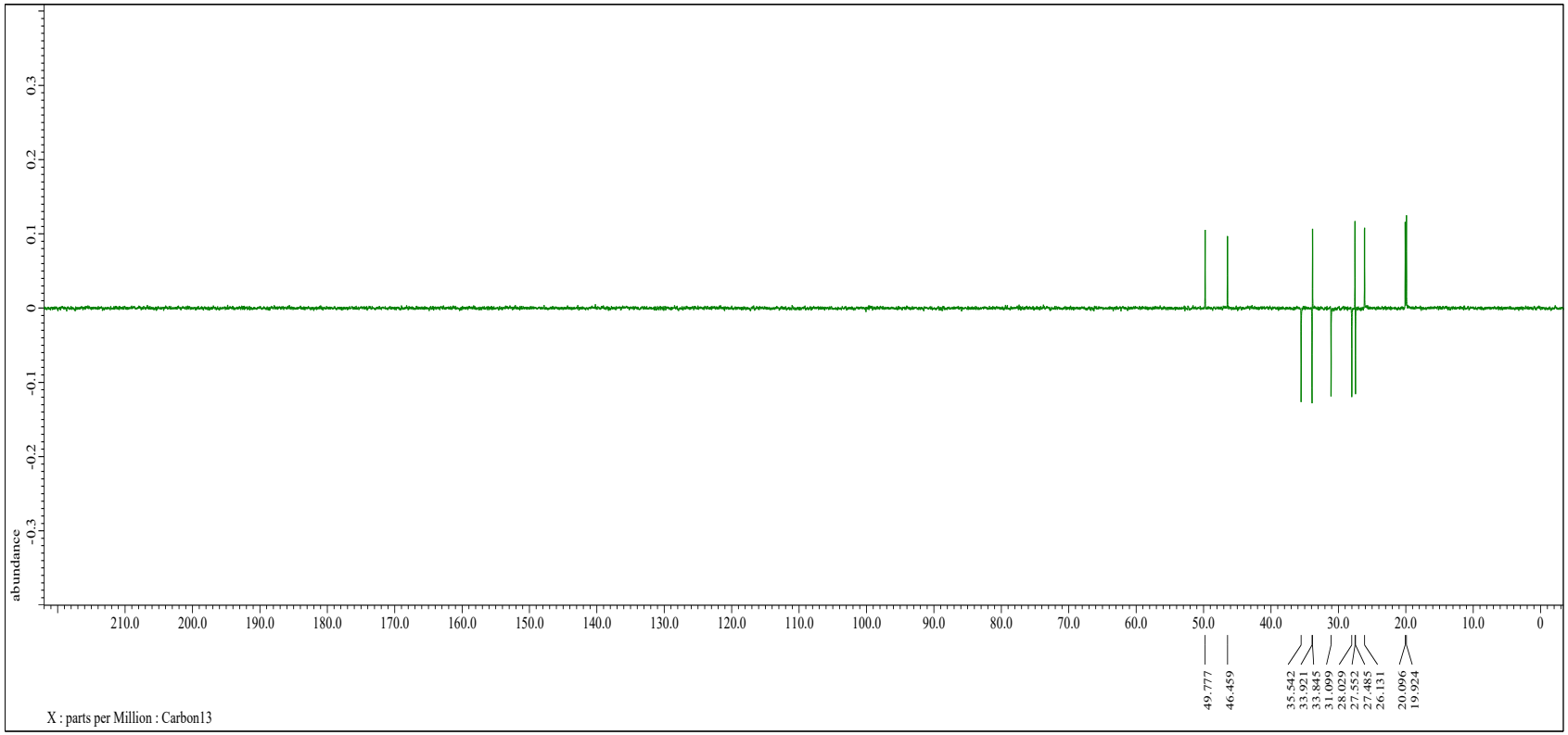


Figure S32. DEPT spectrum of **7** (Recorded in $CDCl_3$)

8. Spectroscopic data for compound 8

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
$C_{15}H_{26}O$	223.2056	233.2047	4.22 / 0.94

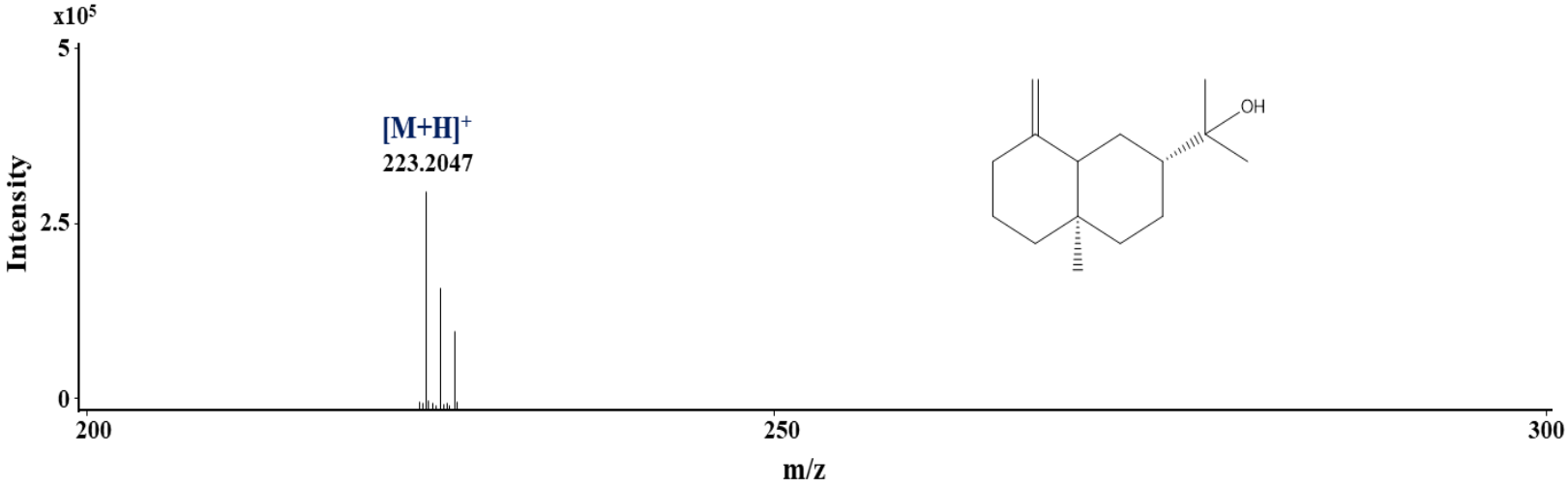


Figure S33. MS spectrum of **8**

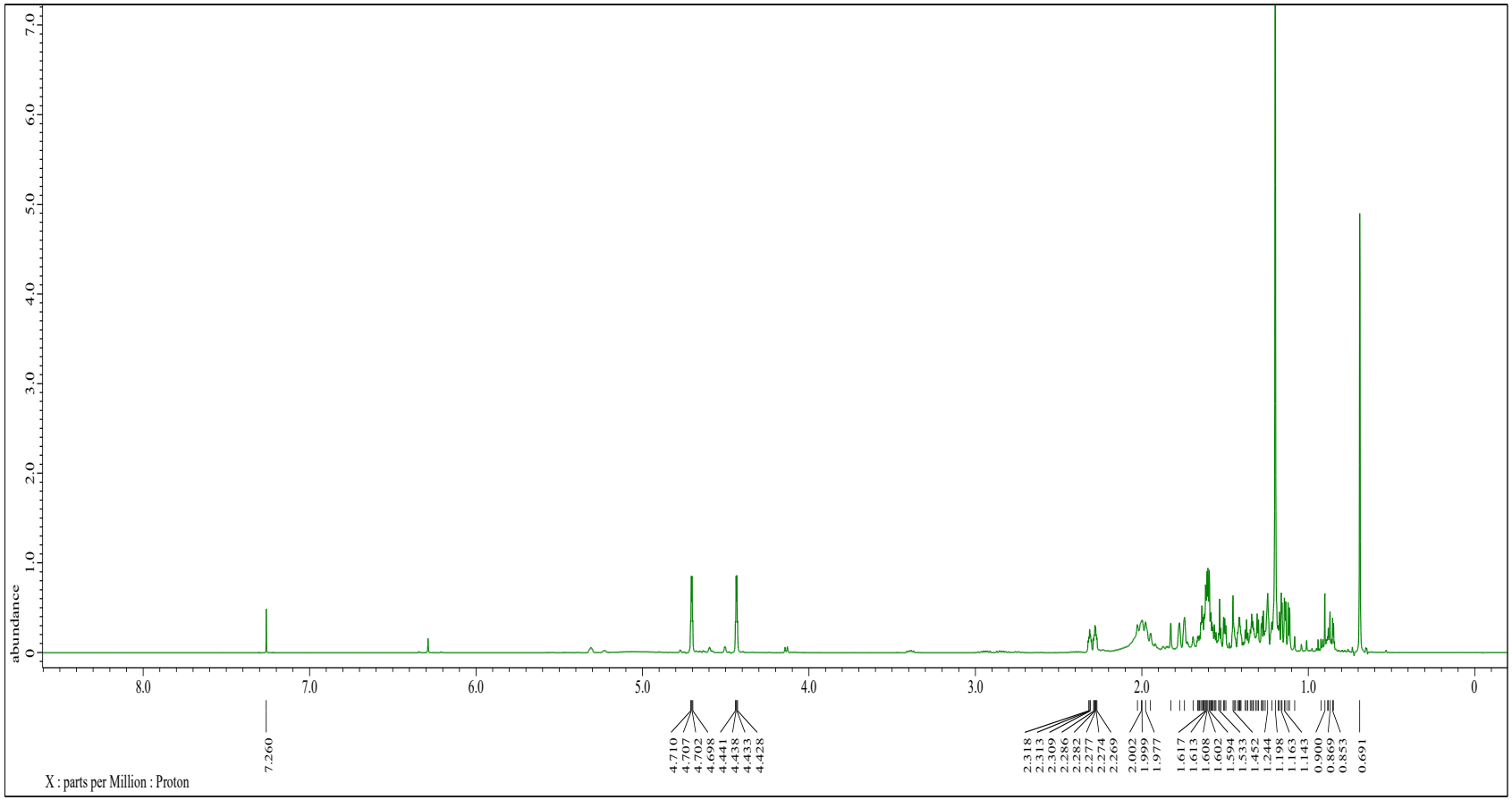


Figure S34. ^{13}C NMR spectrum of **8** (Recorded in $CDCl_3$)

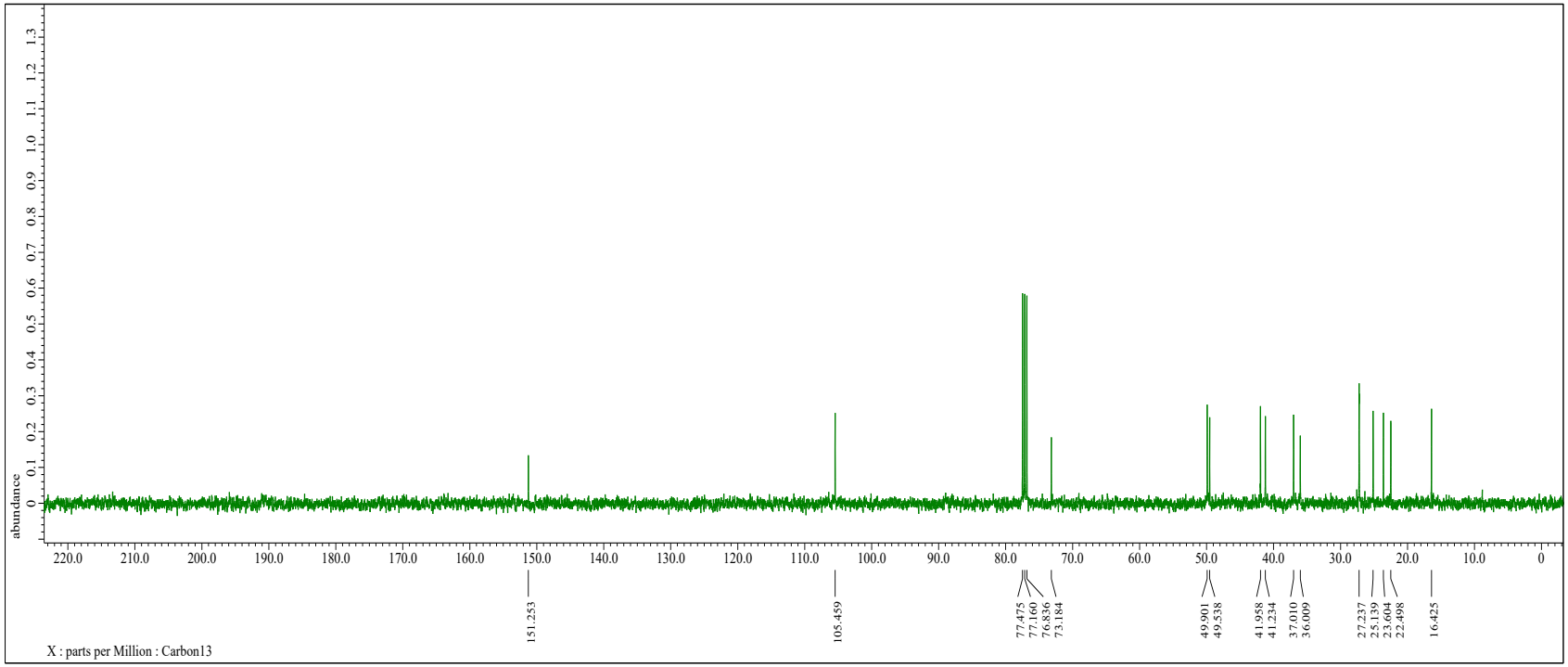


Figure S35. ^{13}C NMR spectrum of **9** (Recorded in $CDCl_3$)

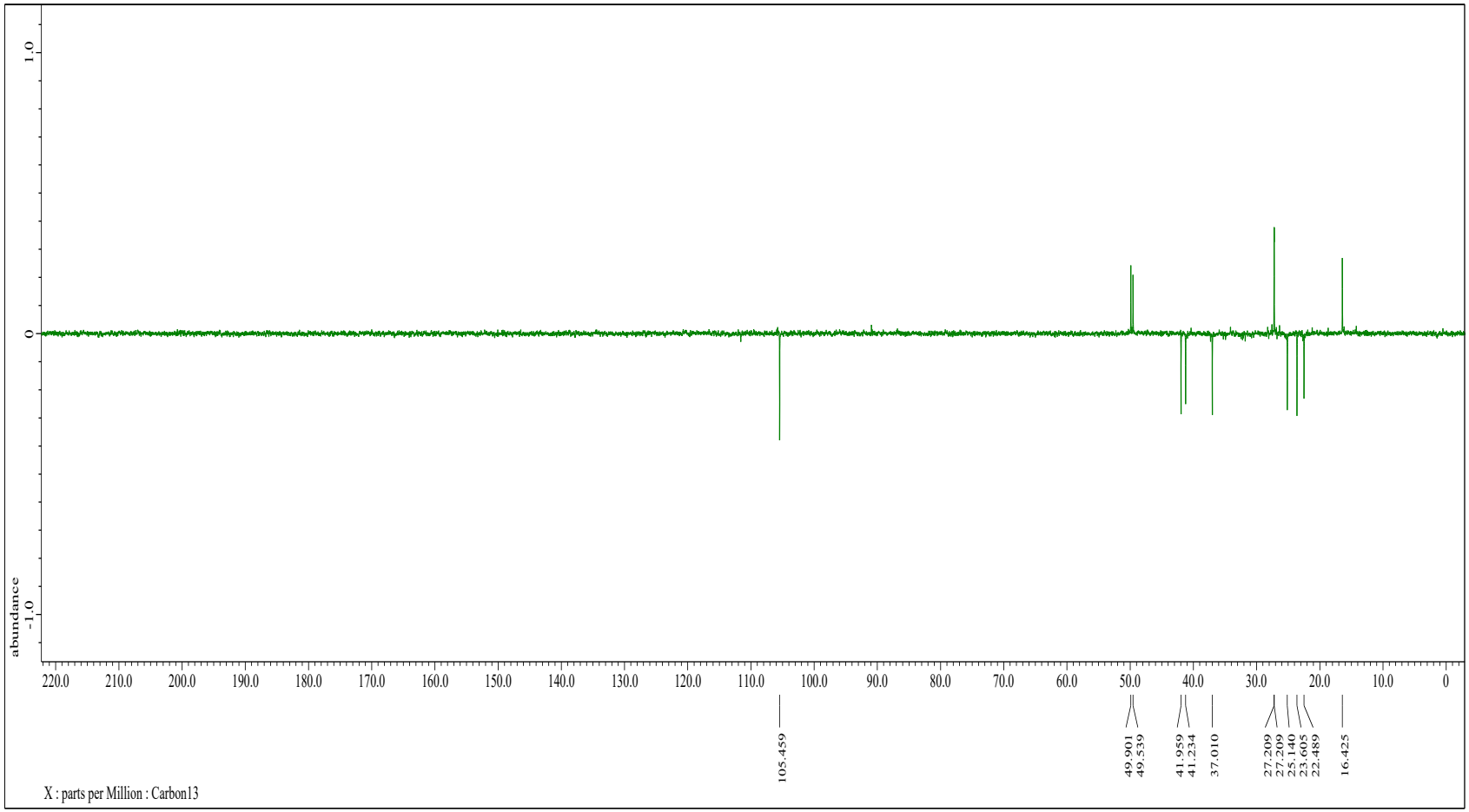


Figure S36. DEPT spectrum of **8** (Recorded in $CDCl_3$)

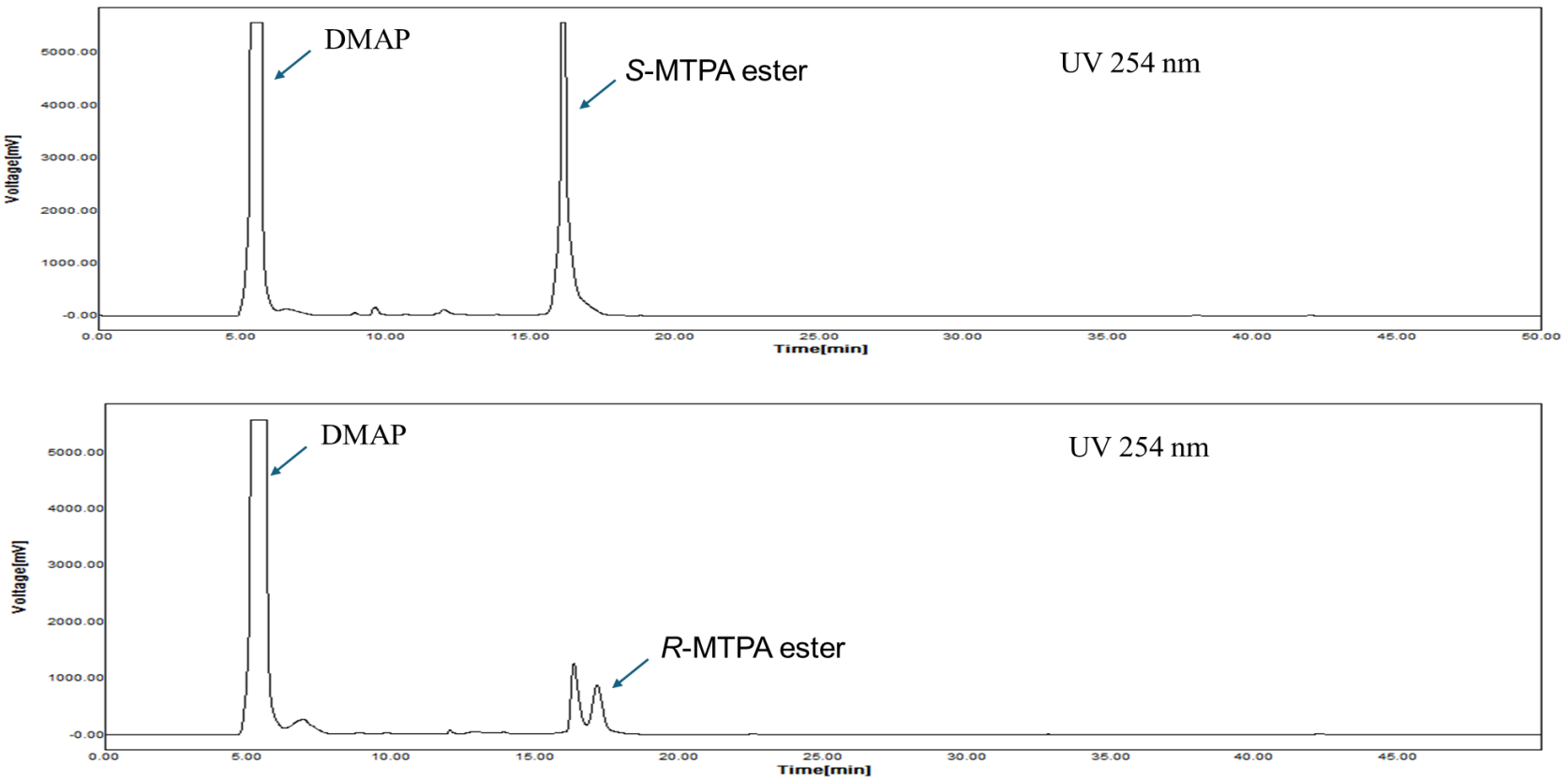


Figure S37. Chromatography Profile of (S) and R-MTPA ester

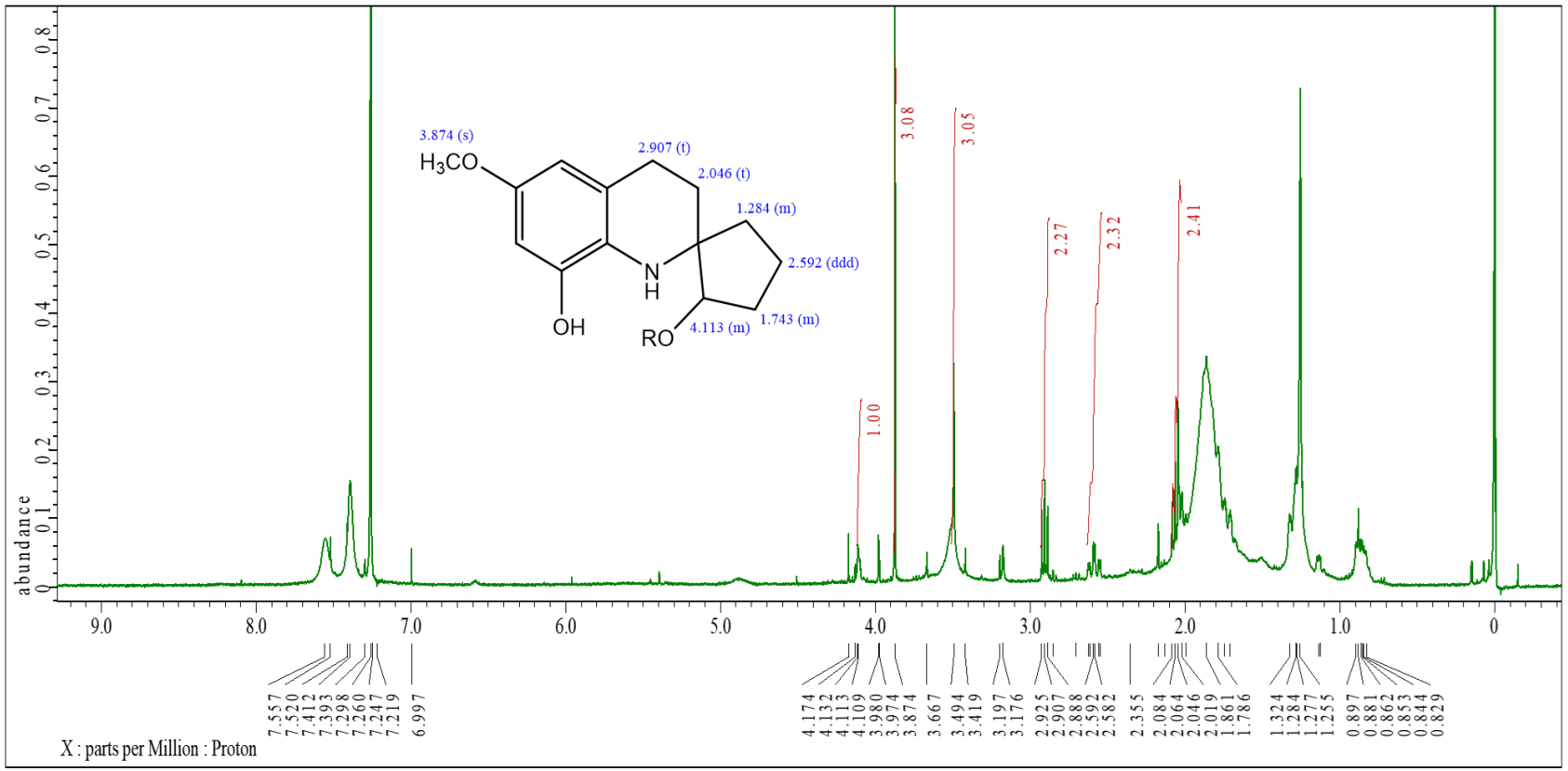


Figure S38. 1H NMR spectrum of 1S (Recorded in $CDCl_3$)

^{1}H NMR ($CDCl_3$, 400 MHz) of (*S*)-MTPA ester of **1**: δ_H 4.113(*m*, H-2), 1.743 (*m*, H-3), 2.592 (*dd*, *J* = 4.4, 13.6, 18.0 Hz, H-4), 1.284 (*m*, H-5), 2.046 (*t*, *J* = 7.2 Hz, H-3'), 2.907 (*t*, *J* = 7.2 Hz, H-4'), 6.977 (s, H-5'), 7.519 (s, H-7'), 3.874 (s, OCH_3).

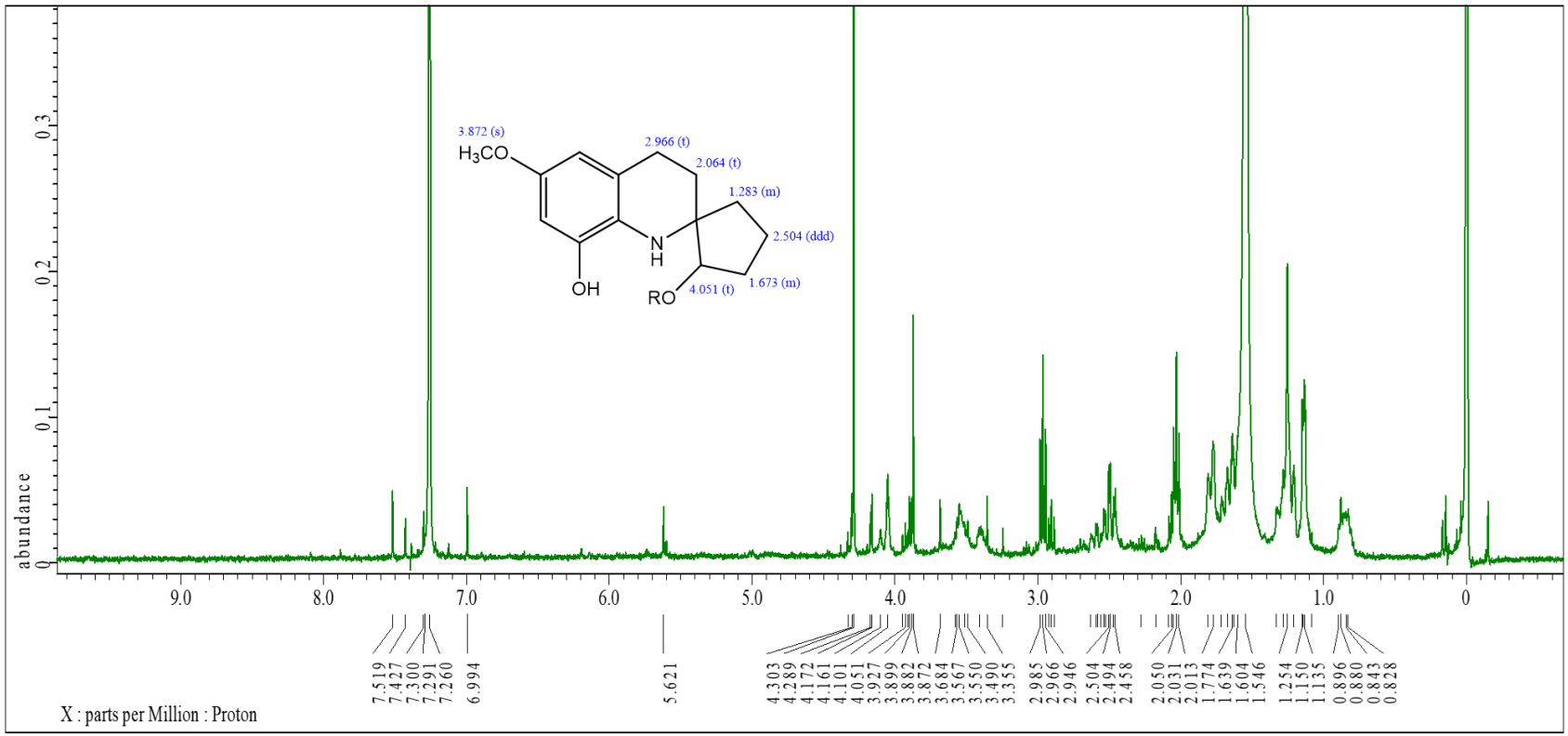


Figure S39. 1H NMR spectrum of 1R (Recorded in $CDCl_3$)

^{1}H NMR ($CDCl_3$, 400 MHz) of (*R*)-MTPA ester of **1**: δ_H 4.051 (*t*, *J* = 3.2 Hz, H-2), 1.63 (*m*, H-3), 2.504 (*dd*, *J* = 4.0, 13.6, 17.6 Hz, H-4), 1.283 (*m*, H-5), 2.064 (*t*, *J* = 7.2 Hz, H-3'), 2.966 (*t*, *J* = 7.2 Hz, H-4'), 6.974 (s, H-5'), 7.519 (s, H-7'), 3.872 (s, OCH_3).

Reference

[1]. Y. Wakahara, T. Noro, J. Sakata, H. Ueda, and H. Tokuyama (2022). Construction of Tetrahydroquinolines with spirocyclic structures at the 4-position, *Heterocycles*. **105**, 438-460.